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1 An “objective” definition of potential vorticity.
2 Generalized evolution equation and application to the
3 study of coastal upwelling instability.

4 Yves Morel^{1,2,*}, Guillaume Morvan^{1,*}, Rachid Benshila^{1,*}, Lionel
5 Renault^{1,*}, Jonathan Gula^{2,*}, Francis Auclair^{3,*}

6 **Abstract**

7 In this paper, we propose a form for potential vorticity (PV), rescaled using
8 the Lorenz’s rearranged density profile, the novelty being that we here take
9 into account its time evolution. We argue this rescaled PV is more repre-
10 sentative of the dynamics, in particular to evaluate the respective impact of
11 mixing and friction on the generation of geostrophic circulation. The im-
12 pact of mixing at global scale, which only modifies the global stratification
13 at rest, is taken into account in the evolution equation of this “objective”
14 definition of PV, in the sense that it scales the PV changes with respect
15 to its effect on the circulation. Numerically, we show that all terms can be
16 calculated coherently using a single computation cell.

17 We illustrate our purpose by studying the instability of coastal upwelling
18 currents, using a numerical model at high resolution. The configuration is a
19 periodic flat channel on the f-plane with vertical walls at the southern and
20 northern boundaries. A constant wind is applied over a fluid at rest with
21 an initial linear stratification. An upwelling current forms at the northern
22 coast. After a few days, instabilities develop and vortices eventually emerge
23 with surface intensified cyclones and subsurface anticyclones. We show that
24 these instabilities and eddies are associated with (rescaled) PV anomalies,

*Corresponding authors
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Email addresses: yves.morel@legos.obs-mip.fr (Yves Morel),
guillaume.morvan@legos.obs-mip.fr (Guillaume Morvan),
rachid.benshila@legos.obs-mip.fr (Rachid Benshila), lionel.renault@ird.fr
(Lionel Renault), jonathan.gula@univ-brest.fr (Jonathan Gula),
francis.auclair@aero.obs-mip.fr (Francis Auclair)

¹LEGOS, University of Toulouse, CNES, CNRS, IRD, UPS, Toulouse, France

²LOPS, University of Brest, CNRS, IRD, Ifremer, IUEM, France

³LAero, University of Toulouse, CNRS, UPS, Toulouse, France

25 triggered by mixing and friction.

26 We describe rescaled PV budgets in a layer bounded between the surface
27 and an isopycnal level. Eulerian and Lagrangian diagnostics allow to analyze
28 irreversible PV production terms, distinguishing the influence of advection,
29 friction (associated with wind stress) and mixing. We find that friction
30 plays the main role, generating negative PV anomalies, while mixing acts to
31 dampen this negative PV production. The association of this negative PV
32 anomaly with the outcropping front leads to the baroclinic destabilization
33 of the upwelling front, creating subsurface anticyclonic vortices and surface
34 intensified cyclonic vortices. Varying the strength of the wind forcing shows
35 that mixing is the most sensitive process, with a net effect that is strongly
36 reduced or even reversed with moderate to weak winds.

When the dynamics is fully turbulent, with filaments and vortices of small sizes, the PV production by mixing and friction is enhanced but the Lagrangian diagnostics are more difficult to analyze, since fluctuations at grid scale become significant and numerical effects – associated with imperfections of the numerical schemes – spoil the PV budget calculation.

37 *Keywords:* upwelling; instability; vortices; potential vorticity; mixing;
38 wind stress.

39 **1. Introduction**

40 The ocean geostrophic circulation is strongly linked to the Potential Vor-
41 ticity (PV) field. The most basic representation of the ocean dynamics is the
42 quasigeostrophic (QG) model (Pedlosky, 1987; Cushman-Roisin and Beck-
43 ers, 2011) , based on the conservation of PV – in adiabatic evolution – and
44 the PV inversion principle (the streamfunction, geostrophic velocity or vor-
45 ticity fields can be inferred from the PV field and boundary conditions). The

46 QG model is based on a simplification of Ertel’s general PV (Ertel, 1942). It
47 has been successfully used in numerous studies and helped to interpret many
48 aspects of ocean dynamics, from the ocean circulation at gyre scale (Rhines
49 and Young, 1982a,b; Luyten et al., 1983; Holland et al., 1984; Rhines, 1986;
50 Talley, 1988; Marshall and Nurser, 1992), to current instabilities (Charney
51 and Stern, 1962), geophysical turbulence (McWilliams, 1984), and isolated
52 vortices (McWilliams and Flierl, 1979; Sutyrin and Flierl, 1994; Morel and
53 McWilliams, 1997).

54 More recently, a few studies have analyzed the influence of non-conservative
55 effects on the evolution of Ertel PV. Haynes and McIntyre (1987) and Haynes
56 and McIntyre (1990) have shown that there are specific constraints on the
57 evolution of PV and that the net PV content in a layer bounded by two isopy-
58 cnic surfaces does not vary. The influence of non-conservative momentum
59 stress at boundaries on PV evolution has also been analyzed theoretically
60 (Thomas, 2005; Morel et al., 2006; Taylor and Ferrari, 2010; Benthuisen
61 and Thomas, 2012, 2013). Since then, several studies have investigated the
62 consequences of diabatic effects on the ocean dynamics from the prism of PV
63 modification, from basin scales (see for instance Hallberg and Rhines, 1996,
64 2000; Czaja and Hausmann, 2009) to meso and submesoscales⁴ (see for in-
65 stance Morel and McWilliams, 2001; Morel et al., 2006; Morel and Thomas,
66 2009; Rossi et al., 2010; Meunier et al., 2010; Thomas et al., 2013; Mole-
67 maker et al., 2015; Gula et al., 2015, 2016, 2019; Vic et al., 2015; Giordani
68 et al., 2017). However, the link between Ertel PV and the dynamics (vor-
69 ticity and velocity fields) is not straightforward, which makes the physical

⁴Mesoscale refers to horizontal length scales close to the internal radius of deformation (10 to 100 *km*) and submesoscale to scales below (1 to 10 *km*).

70 analysis inconvenient.

71 Morel et al. (2019) (see also Assene et al., 2020; Delpech et al., 2020;
72 Aguedjou et al., 2021; Napolitano et al., 2022; Ernst et al., 2023) proposed
73 a rescaled PV, which is calculated taking into account a reference density
74 profile “representative of the background stratification at rest”. The inter-
75 est of the rescaled PV is that it is a generalization of the QG PV. It scales
76 as a vorticity with a reference value at rest equal to the Coriolis parameter
77 (Morel et al., 2019; Assene et al., 2020; Napolitano et al., 2022) and devi-
78 ations of the rescaled PV from its background value at each latitude (also
79 called PV anomalies) are the signature of the vortical geostrophic circulation
80 and can be linked to the dynamics following the QG framework (Morel and
81 McWilliams, 2001; Herbette et al., 2003, 2005; Morel and Thomas, 2009;
82 Le Hénaff et al., 2012). The rescaled PV is conserved for each fluid particle
83 in adiabatic dynamics, but its evolution under diabatic conditions follows
84 similar constraints as the classical Ertel PV (Morel et al., 2019). The gen-
85 erated anomalies are therefore easier to link to the dynamics. Thanks to
86 these properties, the rescaled PV is very useful to analyze the importance of
87 adiabatic and diabatic processes on the generation and evolution of vortices
88 (Assene et al., 2020; Delpech et al., 2020; Aguedjou et al., 2021; Napolitano
89 et al., 2022; Ernst et al., 2023).

90 However, previous studies using rescaled PV have focused on the sub-
91 surface layers and have assumed that the reference density profile does not
92 evolve. Surface layers are subject to strong diabatic processes, so that the
93 reference profile, which is associated with the background stratification and
94 used to define the rescaled PV, may change with time. In addition, outcrop-
95 ping must be taken into account to evaluate the PV budget of the surface
96 layer (bounded by the ocean surface and a deeper isopycnic level). Indeed,

97 outcropping of isopycnic levels at the surface is dynamically equivalent to a
98 positive PV anomaly (Bretherton, 1966; Held et al., 1995; Schneider et al.,
99 2003; Lapeyre et al., 2006; Lapeyre, 2017; Morel et al., 2019). We here pro-
100 pose a new form for the rescaled PV, based on Lorenz’s rearranged profile
101 (Lorenz, 1955) and taking into account its time evolution in case of diabatic
102 mixing. We argue it is the objective form to link PV to the dynamics and
103 measure the respective influence of friction and mixing on the circulation.
104 The evolution equation of this new PV formulation is derived as well as the
105 layer PV budget taking into account surface outcropping. We then illus-
106 trate the use of this general rescaled PV by studying the development of
107 barotropic/baroclinic instabilities along coastal upwelling fronts in a simpli-
108 fied configuration.

109 Coastal upwellings are of particular interest here, since it is known
110 that the developing coastal currents, starting from rest, are subject to
111 barotropic/baroclinic instabilities that generate vortices (Roed and Shi, 1999;
112 Marchesiello et al., 2003; Capet et al., 2004, 2008a,b). Barotropic/baroclinic
113 instabilities can only develop if the PV structure has opposite sign gradients
114 along isopycnic levels (Charney and Stern, 1962; Ripa, 1991). In addition,
115 (cyclo)geostrophic vortices can only exist if their core consists of a local
116 PV anomaly. Thus, Morel et al. (2006) argued that, since the initial PV
117 structure is homogeneous (the ocean is initially at rest), a non-conservative
118 process must be invoked to generate PV anomalies and explain the instabil-
119 ity of upwelling currents and the generation of vortices. They also showed
120 that the friction associated with the wind stress acts differentially along an
121 isopycnic level, leading to a stress curl even with constant wind, which in this
122 case produces systematic negative isopycnal PV anomalies (see also Thomas,
123 2005; Morel and Thomas, 2009). The generated negative PV anomaly then

124 interacts with the surface outcropping, to produce instabilities and vortices
125 of both signs. However, Morel et al. (2006) used a layered model and did
126 not consider diapycnal mixing.

127 We here resume the study of Morel et al. (2006) in a configuration with
128 continuous stratification and taking into account mixing. The wind causes
129 mixing near the surface, so that a mixed layer develops. Since the wind
130 is constant, mixing occurs throughout the domain and modifies the global
131 stratification profile. Away from the coast, the evolution is 1D with an
132 Ekman spiral developing in a deepening mixed layer. The density profile and
133 PV structure evolve, but no isopycnal PV anomalies are generated, so no
134 instability vortices can be generated in this region. Near the coast, variations
135 in stratification and current structures, associated with the development
136 of the upwelling, locally modify the diapycnal mixing, so that isopycnal
137 anomalies can be created by mixing or friction. However, in order to assess
138 the dynamical significance of the generated anomalies, we need to calculate
139 the rescaled PV with a variable reference profile (representing the global
140 stratification at rest at any time).

141 The coastal upwelling configuration is thus a particularly interesting test
142 case for the rescaled PV evolution we propose here. It is also an interesting
143 test in terms of physics, and we will also compare the influence of the wind
144 stress intensity on the PV change and the characteristics of the generated
145 vortices. In section 2, we present the equations, the numerical model and the
146 configuration used in the study. The theoretical framework of the rescaled
147 PV is presented in section 3. We then analyze numerical simulations of
148 upwelling development and instabilities with the rescaled PV in section 4,
149 discussing the effect of friction and mixing with strong and moderate winds.
150 Our results are summarized and discussed in the final section.

151 **2. Equations, numerical model and configuration**

152 *2.1. Equations*

In this paper, we consider the Navier-Stokes equations with Boussinesq approximation:

$$\begin{aligned}\frac{d}{dt}\vec{U} + \vec{f} \times \vec{U} &= -\frac{\vec{\nabla}P}{\rho_0} + \vec{g}\frac{\rho}{\rho_0} + \vec{F} \\ \vec{\nabla} \cdot \vec{U} &= 0 \\ \frac{d}{dt}\rho &= \dot{\rho}\end{aligned}\tag{1}$$

153 where $\vec{U} = (u, v, w)$ is the velocity field, $\frac{d}{dt}\phi = \partial_t\phi + \vec{U} \cdot \vec{\nabla}\phi$, $\vec{\nabla} \cdot \vec{V} = \partial_x V_x +$
154 $\partial_y V_y + \partial_z V_z$ is the divergence of vector field $\vec{V} = (V_x, V_y, V_z)$, $\vec{f} = (0, f_y, f)$
155 is the Coriolis vector (f , its vertical component, is the Coriolis parameter),
156 P is the pressure, ρ is the potential density and $\vec{F} = (F_x, F_y, F_z)$ and $\dot{\rho}$ are
157 terms associated with non-conservative processes for momentum (here the
158 wind stress) and density fields (mixing). They are generally prescribed as
159 diffusive terms $\partial_z(K_\phi \partial_z \phi)$, where ϕ is the velocity or the density field, and
160 the diffusion coefficient K_ϕ is given by some parameterization.

161 *2.2. Numerical model*

162 The oceanic simulations were performed with the Coastal and Regional
163 Ocean Community Model (CROCO, see Debreu et al., 2012), developed
164 around the kernel of the Regional Oceanic Modeling System (ROMS, see
165 Shchepetkin and McWilliams, 2005). CROCO is a free-surface, terrain-
166 following coordinate model with split-explicit time stepping, used here with
167 the Boussinesq and hydrostatic approximations. There are several options
168 for the numerical schemes and here we have chosen a third-order, upstream-
169 biased, dissipative advection scheme, with free slip conditions at lateral

170 boundaries, for horizontal advection of momentum and tracers, (Shchep-
171 etkin and McWilliams, 1998). There is no explicit lateral viscosity in the
172 model.

173 Vertical mixing of momentum and tracers is given by the K-profile pa-
174 rameterization (Large et al., 1994) with a critical Richardson number of 0.3.
175 This closure scheme gives vertical diffusion coefficients for momentum and
176 tracers as a function of wind stress and interior shear (other mixing pro-
177 cesses, associated with internal waves or double diffusion, can be taken into
178 account but are not considered here).

179 *2.3. Upwelling configuration*

180 The configuration is a periodic East-West channel with a flat bottom and
181 vertical walls at the Northern and Southern boundaries (Fig. 1). The chan-
182 nel depth is $H = 1000\text{ m}$ and its width and length are similar $L_x = L_y = 250\text{ km}$.
183 The stratification is initially uniform with a Brundt-Vaisala frequency $N = 5.2\ 10^{-3}\text{ s}^{-1}$.
184 The theory, presented in sections 3.1, 3.2 and 3.3, is valid in general con-
185 figurations taking into account the full Navier-Stokes equations (1), with
186 variable Coriolis parameter and winds, but to simplify the analysis, in the
187 numerical simulations presented here, the Coriolis parameter f and the wind
188 are chosen constant. We fix $f = 7\ 10^{-5}\text{ s}^{-1}$ which gives a first internal radius
189 of deformation $Rd \simeq 23\text{ km}$. The grid step is $\Delta x = 1\text{ km}$. The vertical
190 sigma grid follows Song and Haidvogel (1994) with stretching parameters
191 $\theta_s = 5$, $\theta_b = 0$ and $hc = 30\text{ m}$. We use 80 vertical sigma levels and the
192 vertical resolution ranges from $\Delta z \simeq 1\text{ m}$ at the surface to $\Delta z \simeq 50\text{ m}$ at
193 the bottom. There are 50 layers in the upper 150 m where the dynamics is
194 analyzed.

195 The ocean is initially at rest and we apply a constant West/East wind

196 W (see Fig. 1). The West/East surface stress associated with the wind
 197 is calculated using the bulk formulae $\tau_x = \rho_a C_d |W|W$ (and $\tau_y = 0$),
 198 where $\rho_a \simeq 1.225 \text{ kg.m}^{-3}$ is the air density and $C_d = 0.0012$ the turbulent
 199 momentum transfer parameter. Two different wind velocities are considered,
 200 strong with $W = 8 \text{ m/s}$, and moderate with $W = 2 \text{ m/s}$, corresponding
 201 respectively to $\tau = 0.1 \text{ N/m}^2$ and $\tau = 0.006 \text{ N/m}^2$. Buoyancy (heat
 202 and freshwater) fluxes are not considered here. A quadratic bottom drag,
 203 with a drag coefficient $rdrg2 = 2.10^{-3}$, is used, but it plays no role in
 204 the transformation of PV in the upper layer. We focus on the Northern side
 205 where the upwelling takes place. The downwelling occurring at the Southern
 206 boundary is not studied (PV is also modified in the downwelling area, but
 207 does not lead to instabilities. See Morel et al., 2006, for more details). For
 208 each simulation, we record hourly outputs of all physical fields (velocity
 209 $\vec{U} = (u, v, w)$ and density ρ) but also of the parameterized non-conservative
 210 terms ($\vec{F} = (F_x, F_y, F_z)$ and $\dot{\rho}$).

211 3. Potential Vorticity

212 If the domain was infinite (without Southern and Northern boundaries),
 213 the evolution would be 1D. Indeed, in this case an Ekman spiral devel-
 214 ops and the upper part of the water column undergoes mixing (see Fig. 2
 215 a). The stratification and Ertel PV are modified, with a homogenized up-
 216 per layer overlying a pycnocline with stronger stratification than the initial
 217 stratification. However, there are no horizontal variations of this structure,
 218 and no geostrophic motion is associated with this homogeneous stratifica-
 219 tion change, so the Ertel PV change is not significant in terms of geostrophic
 220 dynamics.

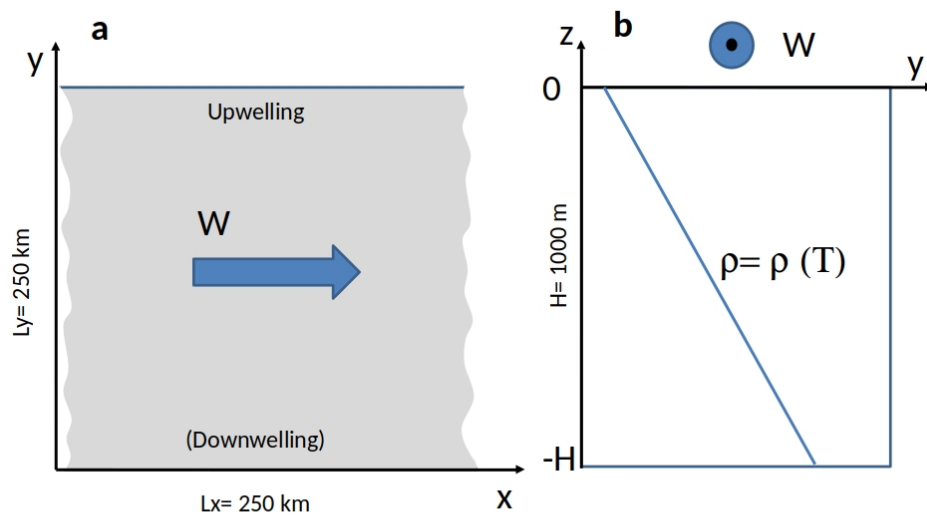


Figure 1: Configuration characteristics, horizontal view (panel a) and vertical section (panel b).

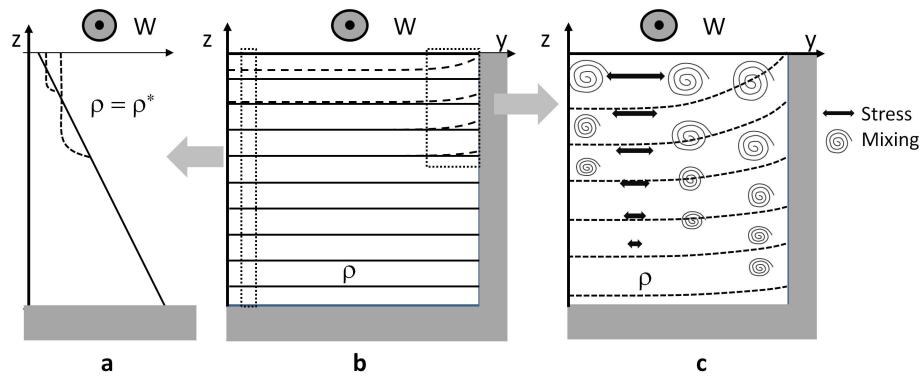


Figure 2: Vertical section of the stratification evolution (panel b). In the open ocean the modifications are close to 1D (panel a), with an Ekman spiral developing in the mixed layer. A pycnocline forms but the stratification below is unchanged. Close to the vertical boundary, where the upwelling develops (panel c), the stratification and current structures are very different. Mixing is modified.

221 In the current configuration, far from the boundaries, the evolution is
 222 close to 1D as depicted above. However, the stratification varies close to the
 223 boundary, where the upwelling develops. Isopycnic levels bend towards the
 224 surface and a vertically sheared geostrophic current develops. Both processes
 225 locally modify the mixing characteristics (Fig. 2 c). As discussed in Morel
 226 et al. (2006), even though the wind stress is constant, the momentum stress
 227 varies vertically, so that a stress curl is created along isopycnic levels bending
 228 towards the surface⁵ (see also section 4.1.2 and Fig. 10).

229 The stress curl and differential mixing create PV anomalies in the up-
 230 welling region and an associated dynamical signal, in particular leading to
 231 destabilization of the upwelling current (Morel et al., 2006). It is therefore
 232 interesting to isolate the PV anomalies generated by diabatic processes that
 233 are truly associated with geostrophic dynamics, and to measure the respec-
 234 tive influence of mixing and friction on the observed dynamics. But such a
 235 measure depends on the definition of PV and the latter has to be carefully
 236 defined to get objective diagnostics. This is a delicate issue that we now
 237 discuss.

238 3.1. An objective definition of Potential Vorticity

As shown by Ertel (1942) (see also Muller, 2006), vorticity is not con-
 served, but a quantity combining vorticity and stratification can be defined
 that is conserved for each particle for adiabatic motions:

$$PV_{Ertel} = (\vec{\nabla} \times \vec{U} + \vec{f}) \cdot \vec{\nabla} \rho \quad (2)$$

⁵Note that the stress parameterization is generally sensitive to the vertical structure of mixing and thus also varies horizontally in the present case, even though the wind stress at the surface is constant.

All dynamical fields (vorticity, velocity and stratification) can be calculated from PV under the simple assumption of (cyclo)geostrophic equilibrium and given boundary conditions. Most studies, using Navier-Stokes or Primitive Equations, invoking PV are based on Ertel PV, including recent studies analyzing the influence of mixing and/or friction. In fact, as already noticed by Ertel, PV is not uniquely defined in the sense that any form of the type

$$PV_{Gene} = (\vec{\nabla} \times \vec{U} + \vec{f}) \cdot \vec{\nabla} G(\rho) \quad (3)$$

-where G can be an arbitrary function- is still a Lagrangian tracer for adiabatic motions. So one may wonder which choice for G is the most objective to define PV. This is particularly important since in case mixing and friction are considered, the evolution equation for PV_{Gene} is

$$\begin{aligned} \frac{d}{dt} PV_{Gene} = \vec{\nabla} \cdot [(\vec{\nabla} \times \vec{F}) G(\rho) \\ + (\vec{\nabla} \times \vec{U} + \vec{f}) \partial_\rho G(\rho) \dot{\rho}] \end{aligned} \quad (4)$$

239 This equation clearly shows that the strength of the PV fluxes associated
 240 with friction (first term on the right hand side) or mixing (second term)
 241 strongly depend on the choice of G . The form of Ertel PV (Eq. 2) with
 242 $G(\rho) = \rho$ has no objective justification apart from its simplicity. In fact,
 243 the interest of PV being its link with the circulation, the adequate form has
 244 to be quantitatively representative of the dynamics, that is to say directly
 245 invertible to estimate the vorticity field. This is not the case of Ertel PV.

246 The proper choice for G can be defined considering a purely barotropic
 247 circulation. Indeed, in this case the dynamics is independent of the vertical
 248 position z (oriented upward), and the background stratification is horizon-
 249 tally homogeneous: $\rho(x, y, z) = \rho^*(z)$ and is also the stratification at
 250 rest. To be representative of the dynamics, PV should correspond to the

251 barotropic vorticity in this case and be independent of z . The only choice
 252 is then that $G(\rho) = Z(\rho)$ where Z is defined using the profile $\rho^*(z)$ so that
 253 $Z(\rho^*(z)) = z$ (the function $Z(\rho)$ corresponds to the vertical position of den-
 254 sity ρ along the reference profile ρ^*). In this case $PV = \partial_x v - \partial_y u + f$ is the
 255 expected absolute vertical vorticity with a value at rest corresponding to the
 256 Coriolis parameter. As argued in previous studies (Delpech et al., 2020; As-
 257 sene et al., 2020; Aguedjou et al., 2021; Napolitano et al., 2022; Ernst et al.,
 258 2023), in the general case, ρ^* should correspond to the stratification at rest,
 259 obtained from the Lorenz’s (Lorenz, 1955) rearranged stratification (see also
 260 Nakamura, 1995; Winters and D’Asaro, 1996). Indeed, in this case only, the
 261 rescaled PV at rest is still given by the Coriolis parameter $PV_{rescaled}^{rest} = f$
 262 and, at first order, the anomaly from this reference corresponds to the quasi-
 263 geostrophic PV, which is again directly linked to the geostrophic circulation.
 264 The link between the geostrophic circulation and rescaled PV is rigorous if
 265 the reference density profile chosen for rescaling correspond to the stratifica-
 266 tion at rest at each time, indicating the necessity to take into account time
 267 evolution of the reference profile. Indeed, Lorenz’s rearranged profile can be
 268 modified by large scale diabatic processes, so that $\rho^* = \rho^*(z, t)$ also depends
 269 on time. For instance, considering again a barotropic circulation for which
 270 large scale ocean/atmosphere fluxes uniformly modify the stratification but
 271 not the dynamics (vertical mixing of momentum does not modify barotropic
 272 circulation), PV should remain equal to the absolute vorticity whatever the
 273 evolution of the background stratification. In addition, in general circum-
 274 stances, mixing and ocean/atmosphere fluxes can destroy or create density
 275 classes in a domain, which can cause problems to evaluate rescaled PV if no
 276 time evolution is considered for the reference profile.

To achieve these properties and be representative of the dynamics at all

times, the objective form for the definition of PV is

$$PV_{rescaled} = \vec{\nabla} \cdot ((\vec{\nabla} \times \vec{U} + \vec{f}) Z(\rho, t)) \quad (5)$$

277 where $Z(\rho, t)$ is a function of both potential density and time and is defined
 278 using the time evolving rearranged Lorenz's profile $\rho^*(z, t)$: Z is chosen
 279 so that at all times $Z(\rho^*(z, t), t) = z$. This is what is chosen in the
 280 present study to compare effects of mixing and friction on the dynamics,
 281 through their associated PV fluxes terms. In our numerical simulations,
 282 the calculation of the reference profile is based on previous work (Tseng and
 283 Ferziger, 2001) with an adaptation associated with the present configuration
 284 (see Appendix A).

285 Interestingly, previous studies, to our knowledge only using non-evolving
 286 Lorenz's profiles, have identified other interesting properties of the rescaled
 287 PV. The PV anomaly proposed by Morel and McWilliams (2001) (see also
 288 Herbette et al., 2003, 2004, 2005; Morel et al., 2006; Morel and Thomas,
 289 2009) is similar to the rescaled PV for adiabatic evolution, but written in
 290 isopycnic coordinate (or for multi-layer shallow water models). This quan-
 291 tity was already shown to be a generalization of the QGPV for primitive
 292 equations (written in isopycnic coordinates) and was used instead of the
 293 classical form because it allows a direct inversion of PV to calculate the
 294 (cyclo)geostrophic circulation. The available potential vorticity, proposed
 295 by Wagner and Young (2015) (see also Early et al., 2021) for the filtering of
 296 internal gravity waves, is similar to the rescaled PV. Gravity waves have no
 297 PV signature along isopycnic surfaces, but in a Eulerian framework when
 298 using the classical form of Ertel PV, the signature of the pycnocline induces
 299 PV variations that are difficult to attribute to geostrophic dynamics or the
 300 displacement of the pycnocline by gravity waves. The use of a rescaled PV

301 for which the PV at rest is uniform (on the f-plane) allows to filter out
 302 the dynamical signature of gravity waves in a Eulerian framework. Finally
 303 Morel and McWilliams (2001) showed that isolated vortices can only have
 304 finite kinetic energy provided the net PV budget is zero in a QG framework.
 305 This theory can be generalized to the Navier-Stokes equations and to frontal
 306 currents (Morel et al., 2019) again provided the rescaled PV is used.

307 *3.2. Generalized evolution equation for the rescaled Potential Vorticity*

The evolution equation of the rescaled PV defined by Eq. 5 is obtained from Eq. 1 following Muller (2006), and we show in Appendix B that it is given by

$$\begin{aligned} \frac{d}{dt} PV_{rescaled} = \vec{\nabla} \cdot (\vec{\nabla} \times \vec{F}) Z(\rho, t) \\ + (\vec{\nabla} \times \vec{U} + \vec{f}) \partial_\rho Z(\rho, t) (\dot{\rho} - \partial_t \rho^* |_{\rho,t}) \end{aligned} \quad (6)$$

or in Eulerian form

$$\begin{aligned} \partial_t PV_{rescaled} = \vec{\nabla} \cdot (\vec{U} PV_{rescaled} \\ + (\vec{\nabla} \times \vec{F}) Z(\rho, t) \\ + (\vec{\nabla} \times \vec{U} + \vec{f}) \partial_\rho Z(\rho, t) (\dot{\rho} - \partial_t \rho^* |_{\rho,t}) \end{aligned} \quad (7)$$

308 where the first term of the right hand side divergence is associated with
 309 adiabatic advection, the second term with friction and the third one with
 310 diapycnal mixing. For the last term, a correction is made to account for the
 311 evolution of the reference profile $\partial_t \rho^* |_{\rho,t} = \partial_t \rho^*(Z(\rho, t), t)$. This evolution
 312 is associated with restratification at global scale and has to be withdrawn
 313 as it has no consequence on the generation of "dynamical" PV anomalies
 314 (see Appendix B). Note that it has to be evaluated along the reference
 315 profile following the density value of the physical domain (not the elevation).

316 Hereafter, PV will refer to the rescaled PV defined by Eq. 5 and whose
317 evolution equation is Eq. 6 or 7.

318 For the upwelling simulation presented above, using the rescaled PV
319 given by Eq. 5 ensures that the PV at rest is unchanged ($PV_{rescaled}^{rest} = f$)
320 and that the isopycnic PV anomalies are representative of the geostrophic
321 dynamics and in particular instabilities.

322 Finally, other forms are sometimes used for the right hand side of Eq. 6,
323 but the present expression has strong similarities with the PV expression in
324 Eq. 5, and is the preferred form for numerical calculations because all terms
325 can be calculated using a single PV grid cell, which also simplifies coherency
326 of PV budgets (see Morel et al., 2019, and Appendix C).

327 3.3. Average PV field in a layer

Since (rescaled) PV represents quasigeostrophic PV at first order, a vertical average of PV in a layer bounded by two isopycnals is informative about dynamical fields. For example, an anticyclonic vortex is associated with a negative PV anomaly, localized in a core within some layer, and the PV budget within the layer is related to the vorticity and stretching fields (see for instance McWilliams and Flierl, 1979; Hoskins et al., 1985; Morel and McWilliams, 1997; Le Hénaff et al., 2012). When the upper bound of the layer is the sea surface, which is generally not an isopycnic surface, an additional term associated with density variations at the surface -outcropping- has to be taken into account when evaluating the PV budget in relation with the dynamics. Indeed, density variation along the surface is equivalent to a Dirac delta sheet of PV that has to be taken into account (Bretherton, 1966; Schneider et al., 2003; Isern-Fontanet et al., 2006; Lapeyre et al., 2006). In this case, the correct calculation for the integrated PV is (Schneider et al.,

2003; Morel et al., 2019; Ernst et al., 2023)

$$\overline{PV} = \frac{1}{h} \left(\int_{z=-h(\rho_{low})}^{z=0} PV \, dz - [(\vec{\nabla} \times \vec{U} + \vec{f}) Z(\rho, t)]_{z=0} \right) \quad (8)$$

328 where $h = h(\rho_{low})$ is the depth of the isopycnic level that defines the lower
 329 boundary of the layer and $Z(\rho, t)$ is the vertical level at density ρ of the
 330 reference profile $\rho^*(z, t)$. The additional term is calculated from velocity
 331 and density fields at the surface ($z = 0$). Note that for an upwelling, the
 332 region where deep isopycnic levels outcrop is equivalent to a positive PV
 333 anomaly ($Z(\rho, t)$ corresponds to the depth of density ρ along the refer-
 334 ence profile and is always negative), which can potentially generate cyclonic
 335 eddies (Bretherton, 1966; Legg and Marshall, 1993; Legg et al., 1996)⁶.

336 4. Numerical results

337 4.1. Reference experiment

338 For the reference experiment, the wind stress is $\tau = 0.1 \, N/m^2$ and the
 339 model is run for 25 days with hourly outputs, starting from rest. Figure 3
 340 shows the evolution of the integrated PV anomaly (using Eq. 8 and a layer
 341 bounded by the isopycnic level $\rho = 1025 \, kg/m^3$ and the surface), surface
 342 vorticity, a vertical section of PV anomaly and vorticity along a South-
 343 North transect. The PV anomaly is obtained from Eq. 5 and withdrawing
 344 the reference PV (f). The vertical sections are taken along the dashed
 345 line shown in the horizontal maps. It is a South-North section located at
 346 $x = 205 \, km$. Note that it crosses the core of a subsurface anticyclonic
 347 vortex at time $t = 21 \, days$ (Fig. 4), whose generation will be studied below.

⁶Physically, if there is no PV anomaly inside the water column but isopycnals outcrop at the surface, internal layers must be stretched and cyclonic vorticity is then created.

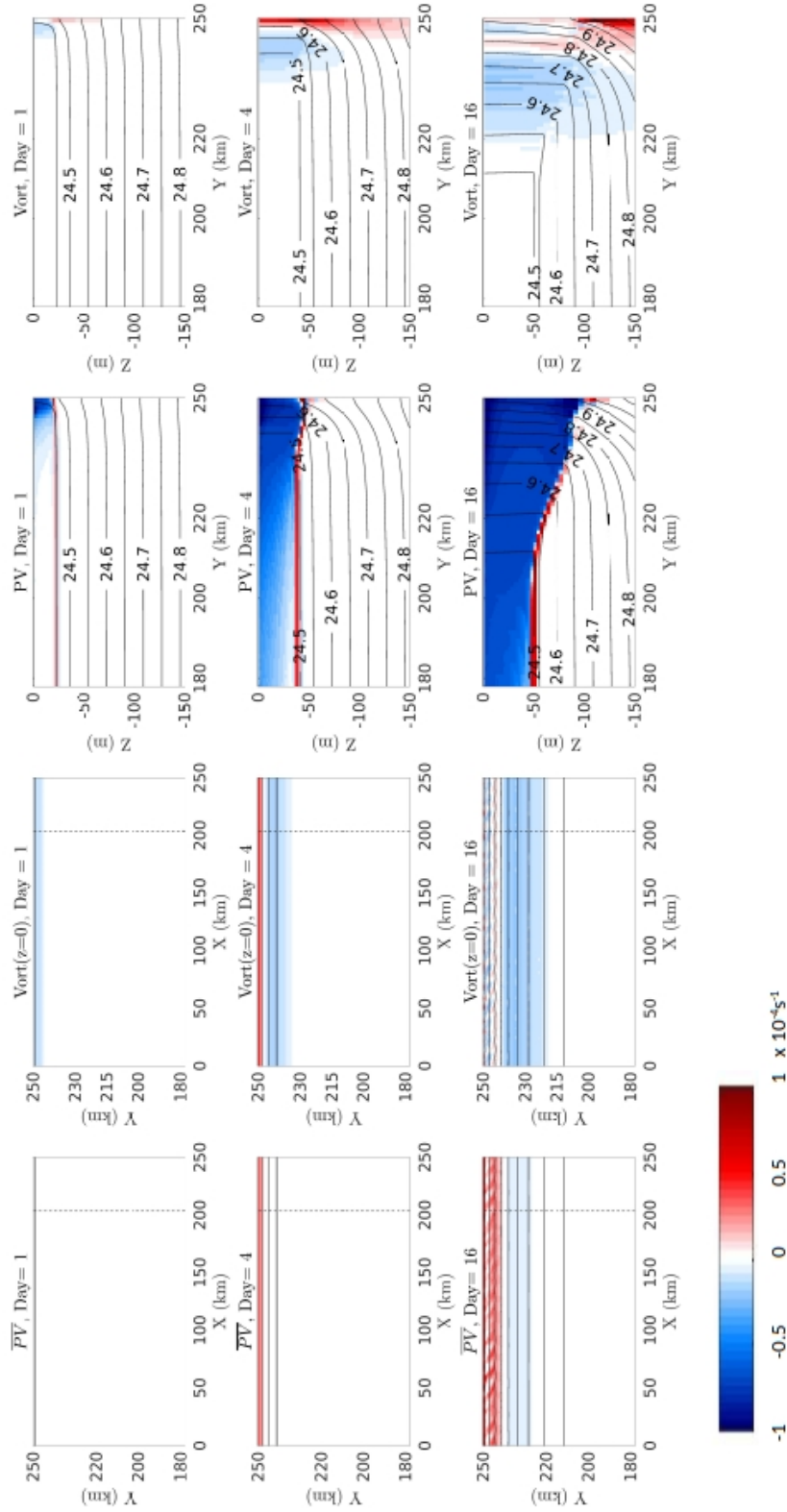


Figure 3: Evolution (days 1, 4, 16. Each day corresponds to a row) of horizontal maps of surface layer averaged PV anomaly \overline{PV} (first column), surface vorticity (second column) and vertical sections of PV anomaly (third column) and vorticity (fourth column). In rows 1, 3 and 4, the solid black contours are associated with isopycnic levels.

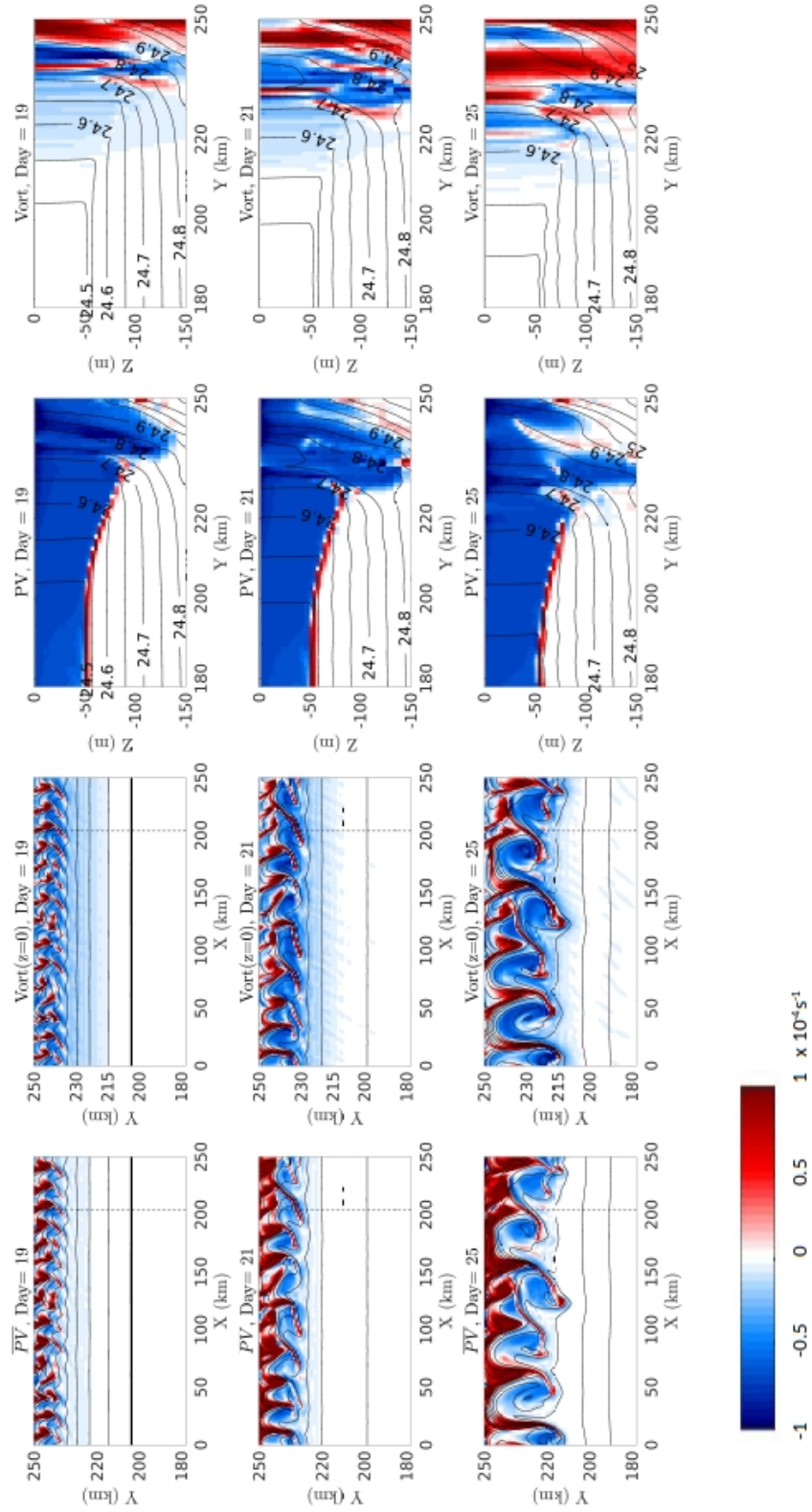


Figure 4: Continued (days 19, 21 and 25).

348 During the early stage, up to day 15, the evolution remains zonal, no
349 instability is visible. From day 15 to 17, short scale instabilities with a
350 maximum length scale of 10 *km* develop, but remain trapped near the
351 coast. Then, from day 18 to 25, new instabilities develop with a domi-
352 nant length scale starting at 20 *km* but evolving to about 40 *km* at day 25⁷.
353 The evolution is similar to that found in Morel et al. (2006), with initial,
354 short scale instabilities developing when the Richardson number becomes
355 smaller than 0.25, corresponding to Kelvin-Helmholtz like instabilities⁸ and
356 larger scale eddies developing from day 18 corresponding to geostrophic
357 barotropic/baroclinic instabilities. At later stages, the merging of eddies
358 also favors the formation of larger scale vortices.

359 Initially, at days 1 and 4, the evolution of the vertical section of PV
360 anomaly and vorticity (columns 3 and 4) is limited to a region close to the
361 northern wall: although mixing modifies the stratification and Ertel PV ev-
362 erywhere in the fluid, the rescaled PV mostly exhibits anomalies where it
363 is dynamically significant, i.e. the generated PV can generate eddies. In-
364 deed, at a later stage, when eddies develop (days 19, 21 and 25) there is
365 a striking correspondence between the surface vorticity and the layer aver-
366 aged PV. In particular, anticyclonic eddies are associated with negative PV
367 anomalies and cyclonic eddies with positive ones. Note that the positive
368 layer PV anomalies are associated with outcropping of isopycnic levels (red
369 areas associated with positive PV anomalies and black contours, associated

⁷All length scales have been evaluated as the dominant wavelength of the x-axis Fourier transform of the surface PV in the upwelling area.

⁸The initial growth of perturbations in KH instabilities is correctly reproduced in primitive equations, but their subsequent evolutions require non-hydrostatic dynamics.

370 with surface density variations, in the first column) and that the order of
371 magnitude of vorticity and PV are similar. Thus, as expected, the (rescaled)
372 PV anomaly can be integrated to evaluate the geostrophic dynamics.

373 As discussed above, outcropping is always associated with equivalent
374 positive PV anomaly (Bretherton, 1966; Schneider et al., 2003). If cyclonic
375 vorticity seems to be mostly associated with the outcropping of isopycnic
376 surfaces, both positive and negative interior PV anomalies are generated, as
377 shown in the vertical section of PV anomaly (third column). They are nec-
378 essarily associated with non-conservative processes. Thus, we now analyze
379 the importance of diabatic mixing and friction in modifying the interior PV.

380 *4.1.1. Eulerian analysis*

381 The simplest diagnostics of PV production by mixing and friction are
382 Eulerian maps of the terms in Eq. 7. As mentioned above, PV, friction
383 and mixing tendency terms can be calculated coherently over a single nu-
384 merical cell following Appendix C, but adiabatic Eulerian advection must
385 be considered too.

386 Figure 5 shows snapshots of all terms appearing in the PV evolution
387 equation (Eq. 7). We focus on the initial stages of the PV evolution when
388 the dynamics remains 2D. The Eulerian PV time derivative at a given time
389 t is obtained from the difference between the PV fields at time $t + 1h$ and
390 $t - 1h$ (using our hourly outputs). Other terms correspond to the tendency
391 terms on the right hand side of Eq. 7 : Advection, Effect of friction and
392 diapycnal mixing. The good coherence between the sum of all terms (second
393 column) and the Eulerian time derivative of PV (first column) confirms the
394 accuracy of our computation. Note that for the present configuration high
395 frequency outputs are necessary to obtain this accuracy. Indeed, using lower

396 frequency outputs (daily or even 12-hourly) can lead to significant discrep-
397 ancies, especially when the geostrophic instability develops, since smaller
398 scale structures appear and are rapidly advected, leading to rapid changes
399 in dynamical fields. Morel et al. (2006) have argued that the effect of the
400 wind stress associated with the friction tendency term (fourth row of Fig.
401 5) should produce negative PV anomalies (see also Thomas, 2005), as long
402 as the stratification remains 2D and with constant wind. From day 15 on,
403 the stratification becomes 3D, positive anomalies appear in the friction ten-
404 dency term (see day 16, fourth row in Fig. 5), possibly generated by the
405 wind stress acting on 3D structures (see for instance Morel and Thomas,
406 2009, for the influence of the wind stress on vortices). Note that the lateral
407 friction could also play a role (even free slip boundary conditions can lead to
408 the generation of PV anomalies, see Morel and McWilliams, 2001) but since
409 horizontal viscosity is implicit, it is not calculated in the friction tendency
410 term and cannot be linked to the positive anomalies seen in Fig. 5.

411 From the impermeability theorem (Haynes and McIntyre, 1987, 1990),
412 one would expect mixing to produce negative PV anomalies in the upper
413 part of the mixed layer – where the fluid is homogenized – and positive ones
414 just below – where a pycnocline appears – (see also Morel and McWilliams,
415 2001). However, with the rescaled PV definition depending on time, this
416 principle is modified. Indeed, in Eq. 7 the time evolution of the reference
417 density (which represents the effect of mixing on a global scale) is discarded
418 from the local diabatic density change, since it does not affect the geostrophic
419 dynamics. Only the diapycnal flux anomaly with respect to the reference
420 density evolution has a dynamical effect and is considered here.

421 This explains the particularly striking fact that over most of the mixed
422 layer, the mixing tendency term remains zero away from the boundary (see

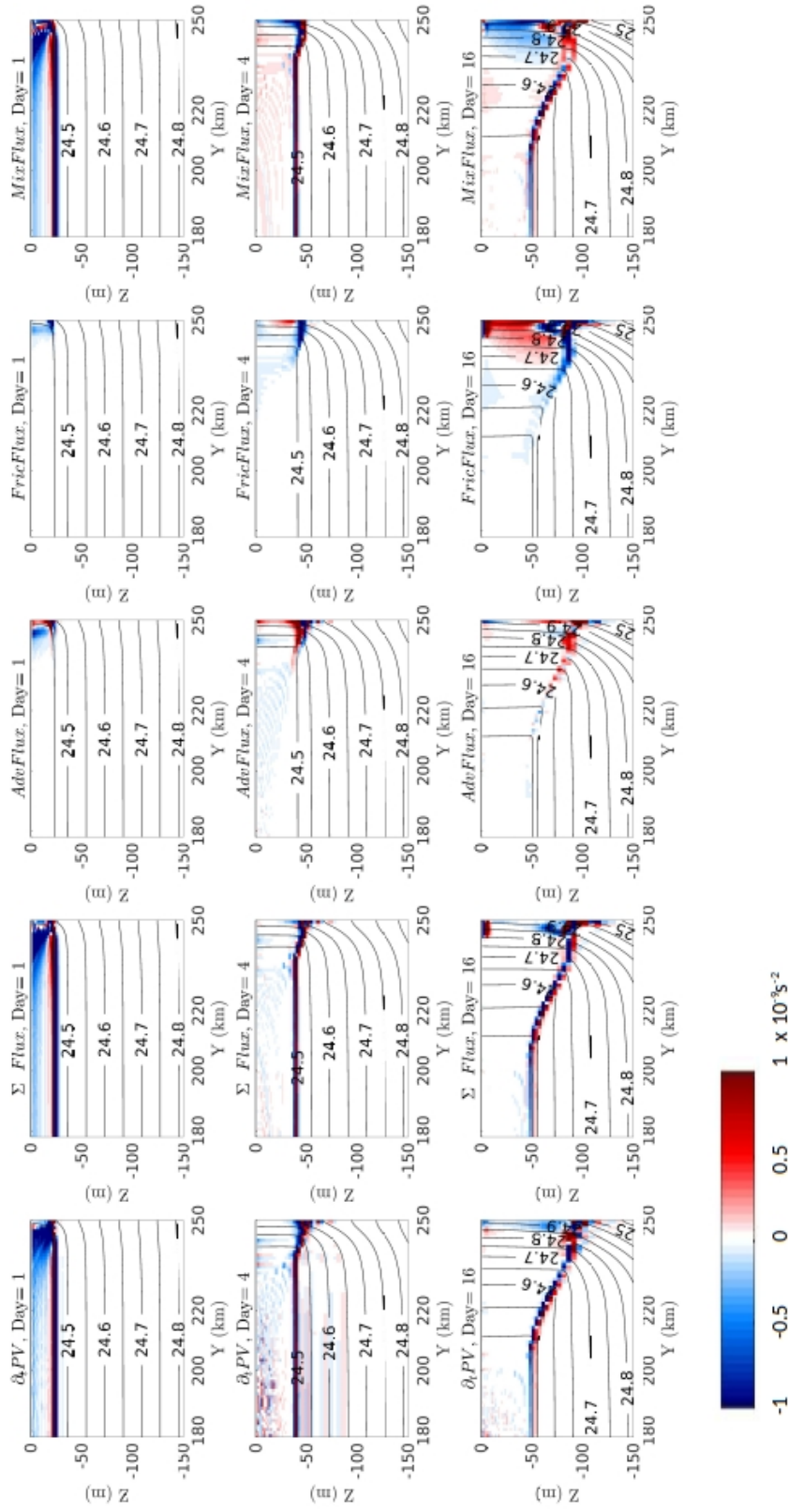


Figure 5: Evolution (days 1, 4, 16. Each day corresponds to a row) of vertical sections, taken along a South-North section located at $x = 205 \text{ km}$, of $\partial_t PV$ (first column), the sum of all right hand side flux terms appearing in the Eulerian PV evolution Eq. 7 (second column), the advective PV flux (third column), the frictional term (fourth column) and the diapycnal mixing term (fifth column).

423 Fig. 5 fifth column), even though mixing continuously modifies the den-
424 sity profile throughout the basin, with a pycnocline that penetrates deeper
425 and deeper throughout the simulation. As discussed above, it is in fact the
426 modification of stratification and velocity in the upwelling area near the
427 coast that generates differential mixing and dynamically significant mixing
428 tendency terms. Since isopycnic levels bend upward, as long as the mix-
429 ing homogenizes a roughly similar depth portion of the water column, we
430 can expect a similar behaviour as described above for the impermeability
431 theorem (the isopycnic levels being mixed in the upwelling region are ini-
432 tially too deep to be affected by the mixing offshore, so the correction term
433 for these isopycnic levels is zero). This is indeed what is seen close to the
434 boundary in the upwelling area (fifth column in Fig. 5). However, the mix-
435 ing associated with rapid offshore advection of denser water at the surface
436 (generating convective mixing) leads to a strong deepening of the mixed
437 layer in the upwelling area and the development of patterns that alter this
438 simple rule, with a complex structure of the mixing tendency term.

439 In fact, it is difficult to evaluate the importance of each process and ten-
440 dency term on the global evolution of PV and the generation of eddies from
441 the Eulerian perspective. In particular, the advective term – which is not
442 associated with PV generation – is of paramount importance. In addition,
443 the tendency terms for mixing and friction often have similar magnitude
444 and extension but with opposite signs, so that the net effect is difficult to
445 evaluate. Note in particular the partial compensation between friction and
446 mixing terms at days 16, when submesoscale structures appear, a process
447 that has been observed and explained in Wenegrat et al. (2018). A better
448 approach is to consider Lagrangian diagnostics, and this is what is presented
449 in the next section.

450 Finally, Fig. 6 compares the previous results (upper panels) to Ertel
451 PV and the associated traditional frictional and mixing productions terms
452 at $t = 1 \text{ day}$ (lower panels). To obtain a scaling for Ertel PV that can be
453 compared to the rescaled PV, we have here used the rescaled form but with
454 the fixed reference profile given by the initial density profile. Indeed, since
455 the initial state has a linear stratification, the non-evolving rescaled PV and
456 tendency terms are proportional to Ertel PV calculations, and quantitatively
457 comparable to the (time evolving) rescaled one. This also allows to illustrate
458 the necessity to use a time evolving reference density profile.

459 As expected, the Ertel PV structure mostly represents the stratification.
460 In comparison with the rescaled PV, the mixing production term is primar-
461 ily marked by the homogenization in the mixed layer and the deepening
462 of the pycnocline over the whole basin, which is not representative of the
463 geostrophic circulation developing in the upwelling area. On the other hand,
464 at this stage, the frictional term for both formulations are pretty close (see
465 Fig. 5). Thus, measuring the respective influence of mixing and friction on
466 the development of the geostrophic circulation using this traditional form of
467 PV can be biased. In the present case negative PV production by mixing
468 production would be over evaluated.

469 *4.1.2. Lagrangian Analysis*

470 A Lagrangian approach is easier to interpret, since we can integrate
471 the global effect for particles forming the core of eddies emerging from the
472 instability of the upwelling current. However, it is numerically more de-
473 manding since it is combined with a tracking algorithm that has some posi-
474 tioning uncertainties associated with spatial and temporal resolution (again,
475 the hourly output is a minimum to achieve good positioning in the rapidly

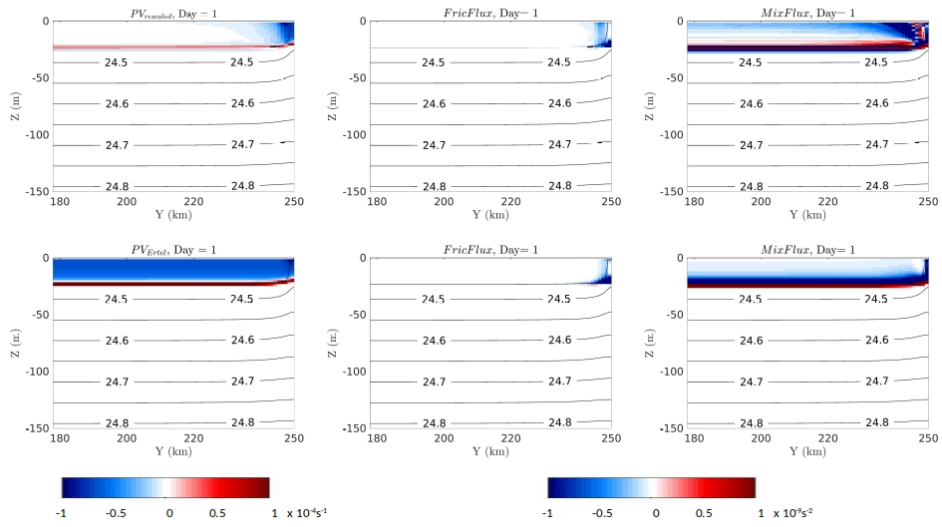


Figure 6: Upper panels : rescaled PV (left panel), frictional term (middle panel) and diapycnal mixing term (right panel) at $t = 1$ day (similar as in Fig. 3 and 5). Lower panels : Ertel PV (left panel), frictional term (middle panel) and diapycnal mixing term (right panel) at $t = 1$ day. Colorscales are given for PV and tendency terms.

476 evolving dynamical structure of the upwelling). The coherence between the
477 PV evolution of a particle and its evaluation from the tendency terms (here
478 only friction and mixing) following the particle in Eq. 6 is thus even more
479 difficult to achieve.

480 We first identify particles with negative PV anomalies in an anticyclonic
481 vortex whose center is located near $x = 205 \text{ km}$, $y = 235 \text{ km}$ at day 21 (Fig.
482 4). 2000 particles were randomly seeded near this position, within a radius
483 of 10 km and with PV anomalies $\delta PV < -10^{-5} \text{ s}^{-1}$. We backtracked them,
484 using time interpolated hourly velocity fields, to obtain their trajectories.
485 The tracking algorithm is the same as that used in Assene et al. (2020).
486 The position of the particles as well as the values of PV and the friction and
487 mixing tendency terms are calculated every 600 s , interpolating the hourly
488 outputs. For each particle, we then integrate temporally the mixing and
489 friction tendency terms obtained from the record of the non-conservative
490 terms (right hand side of Eq. 6) to reconstruct a PV evolution from these
491 diagnostics and we compare it to the PV variations of the particle directly
492 diagnosed from the physical fields. The correspondence is generally good,
493 but given the complexity of the tendency terms, the uncertainties associated
494 with the calculation of trajectories and the hourly sampling, there exist
495 some discrepancies. We then only keep the 1252 particles (representing 63%
496 of the initial 2000 particles) for which the correlation between both PV
497 evolution estimates is greater than 0.9. Figure 7 shows their initial (day 1,
498 in red) and final (day 21, in blue) positions. All particles forming the core
499 of the anticyclonic eddy were initially deeper than their final depth. They
500 also originate from a coastal band that extends about 350 km alongshore
501 (considering the periodicity of the domain) but only 25 km cross-shore, close
502 to the internal deformation radius. Figure 8 shows the PV evolution rate,

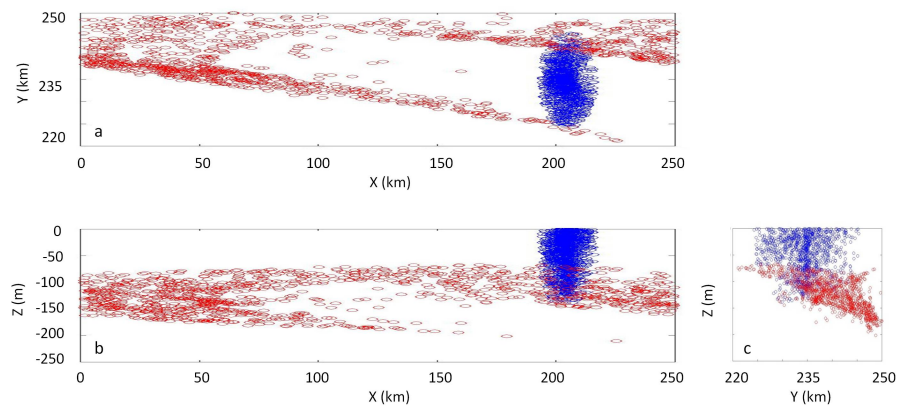


Figure 7: Initial ($t = 1$ day, in red) and final ($t = 21$ days, in blue) positions of selected particles constituting the anticyclonic eddy core. Panel (a) is an X/Y view, panel (b) is a side X/Z view and (c) a side Y/Z view.

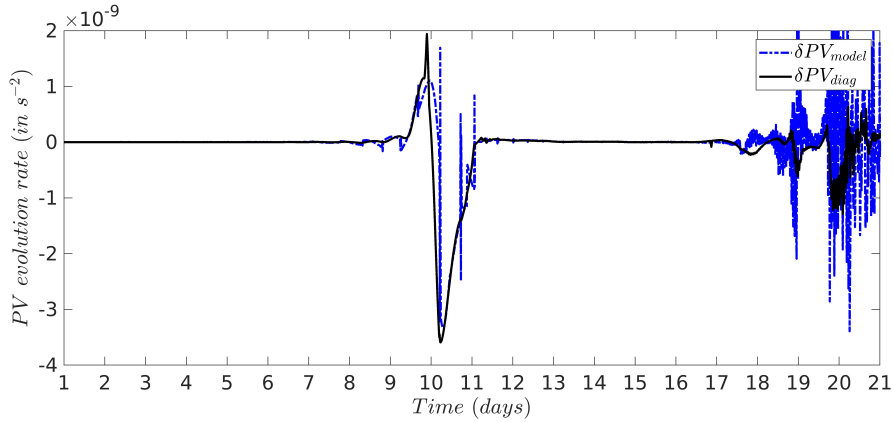


Figure 8: PV evolution rate for a single particle (with maximum correlation between direct PV diagnostic and reconstructed from tendency terms). The blue dashed line corresponds to the calculation from the model PV (calculated using an interpolation of the model PV on the particle’s trajectories) and the black plain line is the diagnostic associated with the sum of friction and mixing tendency terms (again interpolated on the particle’s trajectories).

503 every 600 s, calculated directly from physical fields and diagnosed from the
 504 sum of the friction and tendency terms for a particle with a typical evolution:
 505 the dashed blue curve is obtained from the PV record (calculating $\frac{d}{dt}PV$)
 506 and the plain black curve is the right hand side of Eq. 6, calculated from the
 507 non-conservative terms, along the particle’s trajectories . Note the good
 508 agreement between the two estimates before the circulation becomes 3D and
 509 exhibits small scale variability. This is generally the case for the retained
 510 particles, however, some discrepancies can be seen on the evolution rates, in
 511 particular, the model PV evolution rate exhibits abrupt changes that we do
 512 not see in the diagnosed PV (using tendency terms). But the variations are
 513 close enough to be exploited.

514 In Fig. 9 represents the latitudinal (upper panel) and vertical (middle

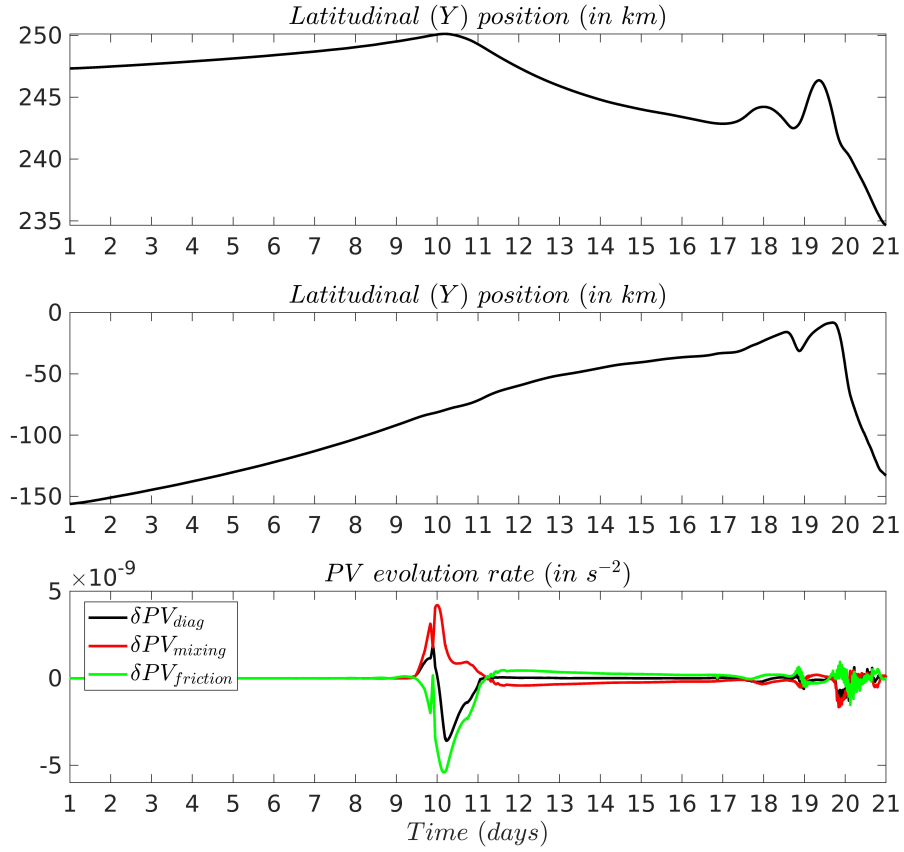


Figure 9: Latitudinal (upper panel) and vertical (middle panel) positions and PV evolution rate (lower panel) for the same particle as in Fig. 8. For the PV evolution rate, the green curve represents the friction tendency term and the red curve the mixing tendency term, the black plain line is the sum of both and is the same as in Fig. 8.

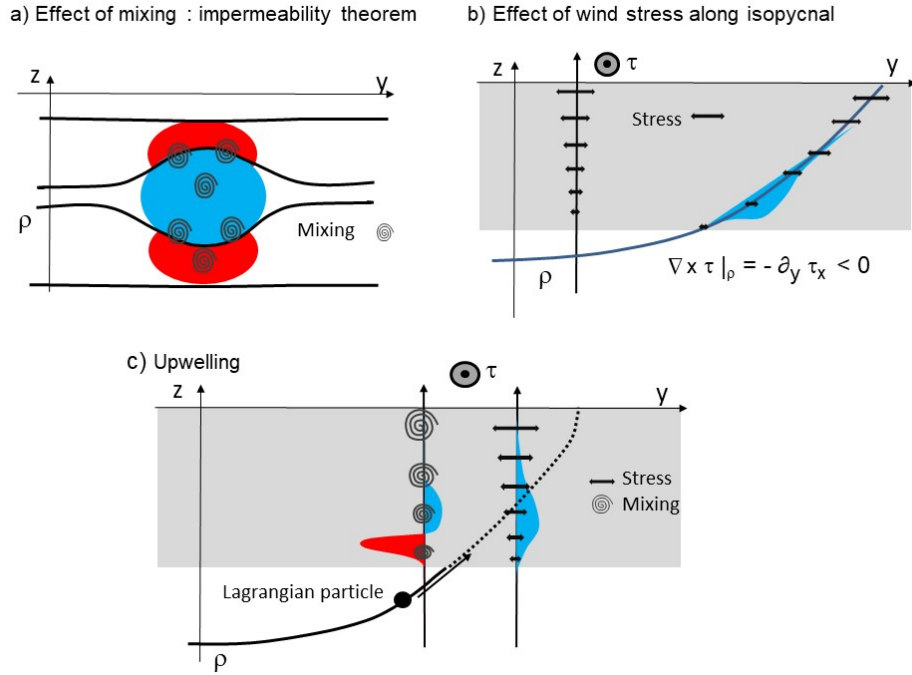


Figure 10: a) Mixing produces negative PV anomalies in region where the stratification is reduced and positive ones in regions where stratification becomes stronger. b) The effect of friction on PV is associated with the curl of the stress, but calculated along an isopycnic surface. The wind stress generally diminishes in amplitude from the surface to the base of the mixed layer. Thus even an homogeneous wind can be associated with a curl, and PV production, along an isopycnal whose vertical position varies. c) In the upwelling case, mixing deepens the mixed layer and thus increases PV at its base and decreases it in the homogenized region. Isopycnic surfaces bend upward and are thus subject to an increasing along-wind stress generating negative curl and negative PV anomalies. In this case, a Lagrangian particle first moves along an isopycnic surface when it is below the mixed layer, and its properties are unchanged. Eventually, it enters the mixed layer where it is subject to friction, which modifies its PV and produces negative anomalies, and mixing, which changes both its density and PV. Mixing generates first positive and then negative anomalies as the particle moves upward.

515 panel) position of the particle and the lower panel shows the respective
 516 contributions from friction (green) and mixing (red) to the global tendency
 517 term (black plain line, already plotted in Fig. 8). The behaviour observed
 518 here is the same for most particles: the particle first moves upward and
 519 Northward – following an isopycnic surface – but is initially not subject
 520 to diabatic forcings and the PV remains unchanged. PV is modified when
 521 the particle enters the base of the mixed layer. As explained in Fig. 10,
 522 it is first affected by mixing, producing positive anomalies (Fig. 10a and
 523 c). Soon after, friction acts too with a negative production rate (Fig. 10b
 524 and c). As the particle moves further upward into the mixed layer, it is
 525 entrained by the surface Southward currents and the mixing PV production
 526 strongly decreases (it can even become negative for some particle) but the
 527 negative production by friction is maintained. The global (friction+mixing)
 528 PV evolution thus evolves from positive to negative with longer and stronger
 529 negative production, so that the final PV anomaly of the particle is generally
 530 negative. After this strong modification episode when entering the mixed
 531 layer, the particle is subject to a phase where mixing and friction production
 532 equilibrate so that its PV value is maintained. After day 18, when the
 533 instability develops and produces small scale variability, marked by higher
 534 frequency changes in horizontal and vertical positions, PV evolves again but
 535 the physics of this phase is more difficult to explain since there are strong
 536 numerical uncertainties.

537 Figure 11 shows the mean evolution calculated from the 1252 selected
 538 particles with high correlation. The mean PV anomaly gradually decreases
 539 (plain black and dashed blue curves) and the final value is strongly nega-
 540 tive (the PV anomaly is $\delta\overline{PV} \simeq -6.10^{-5}s^{-1}$). Note that after day 18,
 541 discrepancies appear between the model PV (blue dashed curve) and the

542 PV diagnosed from the tendency terms (black plain curve). As explained
543 above, the development of the instability generates small, rapidly evolving
544 eddies. Implicit diabatic terms, associated with imperfections of the numer-
545 ical schemes at the grid scale and the limited (hourly) output frequency used
546 for our diagnostics, corrupt the PV budget. However, the development of the
547 PV structure responsible for the initial instability is correctly represented
548 before the emergence of small scale 3D structures, During this period, fric-
549 tion produces negative PV anomalies (green curves in Fig. 11). Although
550 it produces both positive and negative anomalies, the effect of mixing is
551 to dampen the effect of friction by producing a net positive anomaly (red
552 curves) at a rate that is – on average – similar in amplitude in this refer-
553 ence experiment. For particles entering the lateral boundary layer, lateral
554 friction can also affect the friction tendency term with an effect that can
555 be more difficult to predict as it depends on details of the velocity varia-
556 tions near the wall and the horizontal viscosity scheme used in the model
557 (D’Asaro, 1988; Morel and McWilliams, 2001; Akuetevi and Wirth, 2015;
558 Morel et al., 2019), but the general negative friction tendency term observed
559 here is mostly associated with the effect of the wind stress and its redistribu-
560 tion in the surface mixed layer. Testing with different anticyclonic vortices
561 or changing the selection criterion for retained particles does not change our
562 findings.

563 As can be seen from Fig. 4, cyclonic structures are constituted of smaller
564 vortices and filaments and are not as well defined as anticyclonic vortices. It
565 is also clear that the interior PV anomaly is mostly negative, although there
566 are traces of positive PV anomalies on vertical sections (third column in Fig.
567 3). We selected areas with positive interior PV anomalies and performed
568 a similar Lagrangian analysis (again backtracking 2000 particles from day

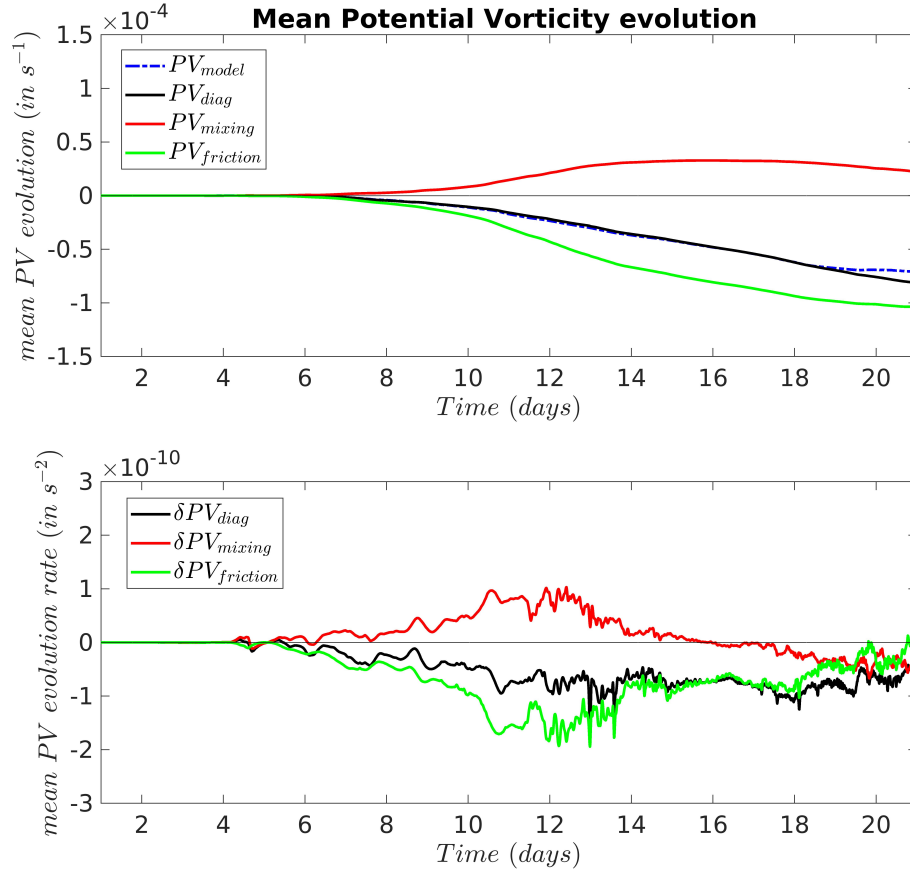


Figure 11: Mean PV evolution (upper panel) and evolution rate (lower panel) for all 1178 selected particles, constituting the anticyclonic eddy core (Fig. 7). For the upper panel, the blue dashed line corresponds to the PV anomaly of the model (calculated from the PV values of all selected particle at a given time from which we withdraw f), the green curve is obtained from the time integration of the friction tendency term and the red curve from the mixing tendency term, the black plain line is the sum of the integrated tendency terms and is to be compared to the blue dashed curve. The lower panel is similar but for the tendency terms (evolution rate).

569 21). We found that the positive interior PV anomaly of particles constitut-
 570 ing cyclonic eddies is determined during the last days of the evolution, i.e.
 571 after day 18, when the instability starts to develop. The criterion for par-
 572 ticle selection had to be modified and the minimum correlation coefficient
 573 between model and diagnosed PV evolution was lowered to 0.7 to keep a
 574 few hundred particles. The mean PV anomaly of the particles constituting
 575 cyclonic eddies at day 21 was $\delta\overline{PV} \simeq +1.5 \cdot 10^{-5} s^{-1}$, much lower than for
 576 anticyclonic structures (in absolute value). As mentioned above, the exten-
 577 sion of the eddies is also much smaller, but it is also constituted of different
 578 subcores, i.e. disconnected parts associated with local maximum. In fact,
 579 eddies associated with positive vorticity or average PV anomalies are domi-
 580 nated by the surface outcropping signature, under which the positive interior
 581 PV anomaly eddies, generated during the development of the geostrophic
 582 instability, align. As seen before, mixing creates the positive PV anomalies
 583 at the base of the mixed layer, but during the late stage of the evolution,
 584 friction can also produce positive PV. Indeed, we have seen (see Fig. 10)
 585 that, during the upwelling development phase, the decrease of the stress
 586 from the surface and the upward bending of isopycnals is associated with a
 587 negative curl of stress along isopycnic levels, which explains the formation
 588 of negative PV anomalies by friction. If the isopycnal bends downward,
 589 which is the case when the instability develops and vortices emerge, the curl
 590 becomes positive and positive PV anomalies is then produced by friction
 591 (Morel et al., 2006).

592 *4.2. Sensitivity to wind stress*

593 We now evaluate the sensitivity of the PV change to the wind stress.
 594 As noted above, although we have considered a constant wind, the stress

595 along isopycnic levels is locally modified in the upwelling region, since it
596 depends on the isopycnal position, velocity shear and local vertical viscosity
597 coefficient (Morel et al., 2006, 2019).

598 We lowered the wind intensity with $W = 2 \text{ m/s}$ corresponding to a
599 stress of $\tau \simeq 0.006 \text{ N/m}^2$, 16 times smaller than before, and performed the
600 same analysis on PV evolution. Figure 12 is similar to Fig. 3 and shows
601 the evolution of vertically averaged upper-layer PV anomaly, surface vor-
602 ticity, vertical section of PV anomaly, and vorticity along a South-North
603 transect at $x = 205 \text{ km}$. Due to the lower forcing wind stress, mixing is
604 less intense and the layer affected by mixing and wind stress is shallower.
605 The upper layer over which PV is averaged is now bounded by the isopy-
606 cnic level $\rho = 1024.6 \text{ kg/m}^3$ and the surface. The evolution is also slower
607 than before with some peculiarities. First, Kelvin-Helmholtz like instabili-
608 ties start at day 22 with several sequences until about day 37 when longer
609 wavelength geostrophic instabilities develop, evolving into mesoscale struc-
610 tures after about 70 days. The layer PV and the surface vorticity structures
611 are still strongly connected, but the patterns are different compared to the
612 reference experiment with smaller and weaker anticyclonic vortices. The
613 vertical sections of PV anomaly show little trace of positive PV anomalies
614 in the interior during most of the evolution, and it appears only at the stage
615 of fully developed turbulence (see the vertical section of PV at day 90, Fig.
616 12 last line, third row). Finally the isopycnic levels (black contours on the
617 vertical sections) are less steep in the upwelling region, indicating that the
618 fluid remains more stratified.

619 In Fig. 14 we plot the PV tendency terms associated with friction and
620 mixing and their sum. Before the development of the geostrophic instability,
621 PV anomalies generated by mixing show a different pattern for this lower

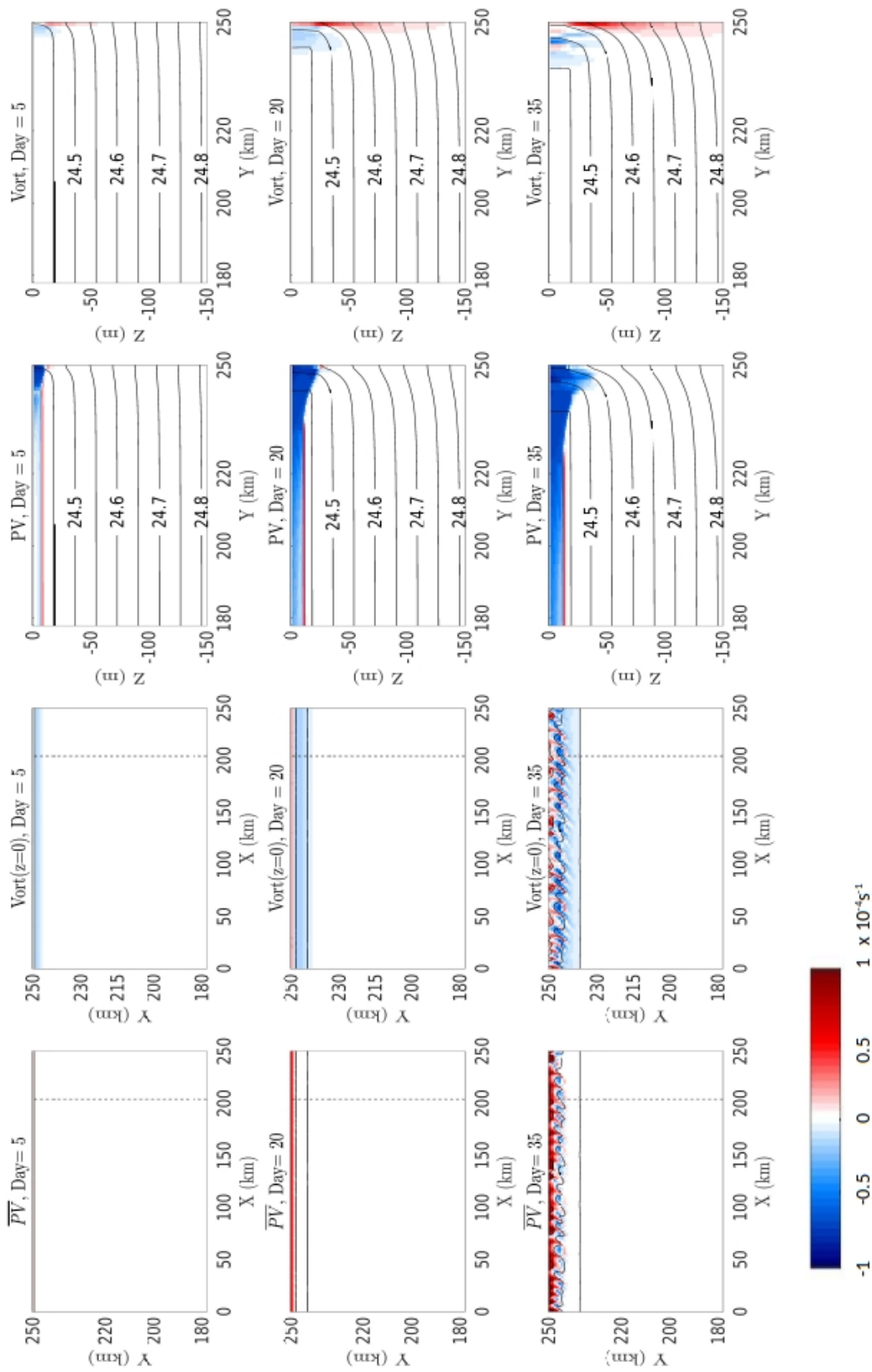


Figure 12: Evolution (days 10, 20, 35 for the experiment with a wind stress reduced to $\tau = 0.006 \text{ N/m}^2$. Each day corresponding to a row) of horizontal maps of surface layer average PV anomaly (first column), surface vorticity (second column) and vertical sections of PV anomaly (third column) and vorticity (fourth column). The PV anomaly is obtained by withdrawing the reference PV, that is f . The vertical South-North sections are taken along the dashed line represented in the horizontal maps (at $x = 205 \text{ km}$). Note that it crosses the core of an anticyclonic subsurface vortex at day 46. In rows 1, 3 and 4, the solid black contours are associated with isopycnic levels.

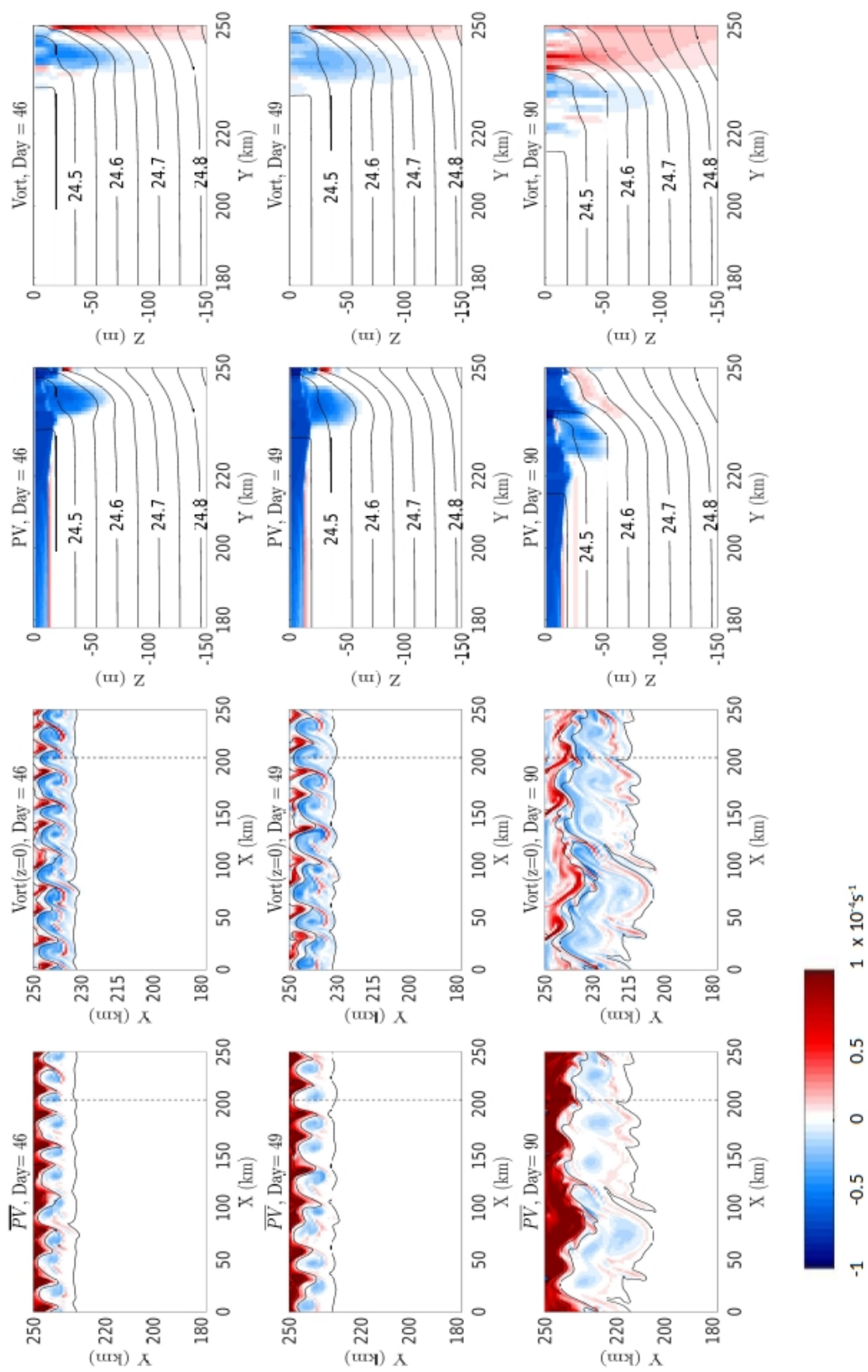


Figure 13: Continued (days 46, 49 and 90).

622 stress simulation, with sometimes a layer of negative PV production below
623 the positive one (row 1 and 2 of MixFlux, third column), which is inverted
624 compared to Fig. 5. The influence of the correction term, associated with
625 the evolution of the reference profile, is more important here: the presence of
626 the upwelling close to the coast generates a stronger stratification that is not
627 compensated by the shear, and mixing diminishes in the upwelling region
628 in comparison to the rearranged profile. This shows that nonlinearities and
629 details of the evolution, associated with the mixing closure scheme, can
630 lead to strong differences for the -rescaled- PV production and subsequent
631 dynamics.

632 As for the reference experiment, 2000 particles were seeded into the anti-
633 cyclonic structure observed in the vertical section at day 46, whose center is
634 located at $x = 205 \text{ km}$ and $y = 242 \text{ km}$. These particles were backtracked
635 to their initial positions while computing their PV and the PV tendency
636 terms at their positions every 600 s . Using a similar selection criterion as
637 for the reference experiment (correlation between the PV evolution and that
638 reconstructed from the tendency terms above 0.9) about 1100 particles were
639 retained. Figure 15 is similar to Fig. 11 and shows the evolution of the
640 mean PV anomaly from the model (blue dashed line), the integration of
641 the friction tendency term (green line), the mixing tendency term (red line)
642 and the sum of both tendency terms (black line). There are striking differ-
643 ences with the reference experiment. First, both friction and mixing lead to
644 negative PV production on average, but mixing has a modest effect; most
645 of the variability is associated with friction, before the development of the
646 geostrophic instability and vortex formation. The rate of PV production is
647 also about 10 times weaker for friction or mixing. Another interesting as-
648 pect is that the analysis of individual particles (not shown) shows that after

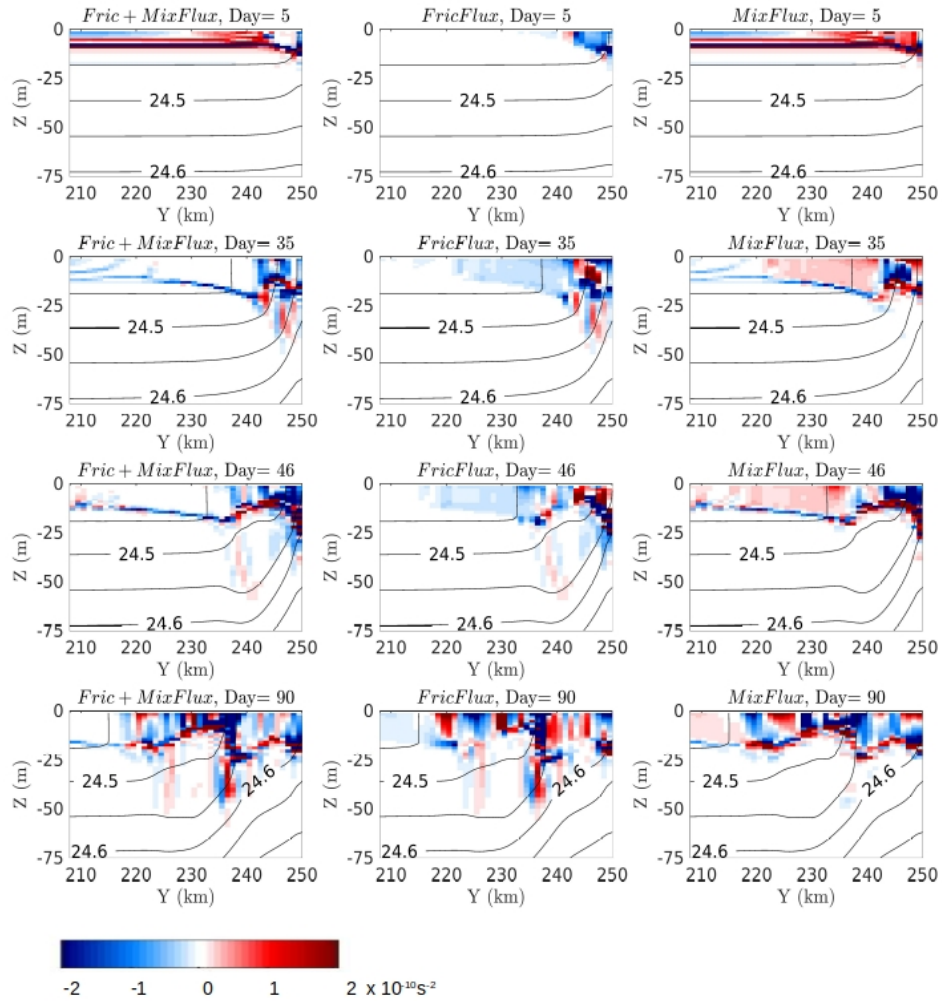


Figure 14: Evolution (days 10, 35, 46 and 90. Each day corresponding to a row) of vertical sections, taken along a South-North section located at $x = 205 \text{ km}$, of the sum of diabatic tendency terms (first column), the frictional term (second column) and the diapycnal mixing term (third column) for the sensitivity test with a reduced wind stress ($\tau = 0.006 \text{ N/m}^2$).

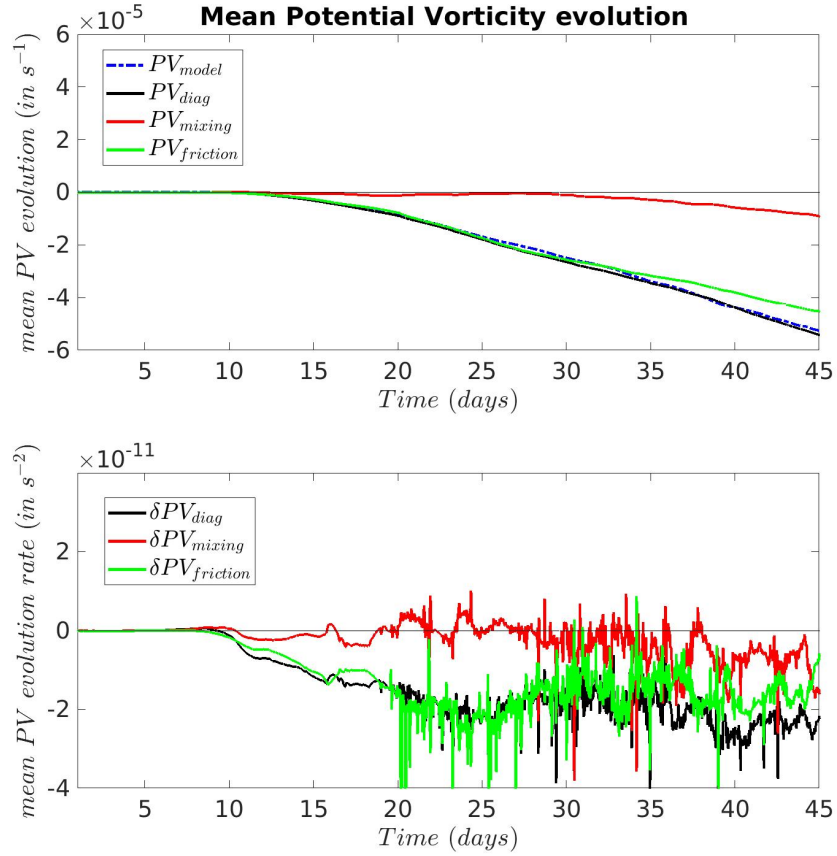


Figure 15: Mean PV evolution (upper panel) and evolution rate (lower panel) of all 1083 selected particles forming the anticyclonic eddy core (Fig. 7) in the experiment with the wind stress reduced to $\tau = 0.006 \text{ N/m}^2$. For the upper panel, the blue dashed line corresponds to the PV anomaly of the model (calculated from the PV values of all selected particles at a given time from which we remove f), the green curve is obtained from the time integration of the friction tendency term and the red curve from the mixing tendency term, the black solid line is the sum of the integrated tendency terms and is to be compared with the blue dashed curve. The lower panel is similar, but for the tendency terms (evolution rate).

649 day 40, small scale processes spoil the PV budget for individual particles,
650 but the mean evolution remains quite close to the estimated PV evolution
651 (black and blue dashed curves in the upper panel of Fig. 15), whereas in
652 the reference experiment, this leads to a bias.

653 **5. Summary and Discussion**

654 In the present paper, we advocate the use of a form of PV, rescaled by
655 the time-evolving Lorenz's rearranged density profile (Lorenz, 1955; Naka-
656 mura, 1995; Winters and D'Asaro, 1996). The proposed PV is the only form
657 able to associate PV to the absolute vorticity for barotropic circulation. In
658 general circumstances, it is also a generalization of the QG PV and is easily
659 connected to the (cyclo)geostrophic circulation. We thus argue that this
660 form of PV provides an objective evaluation of the effect of mixing and fric-
661 tion on the generation of PV. Its time evolution equation is derived and
662 it is shown that global changes in stratification must be removed from the
663 mixing production term, following isopycnal levels. The proposed form of
664 PV and its evolution equation are valid in general (realistic) circumstances
665 for the Navier-Stokes or Primitive equations. We believe this form has to be
666 chosen when interpreting PV evolution in terms of dynamics (that is when
667 using the inversion principle, relating PV to the circulation), especially to
668 evaluate the respective influence of mixing and friction. Equation 6 shows
669 that the objective rescaling of PV may lead to different interpretation de-
670 pending on the characteristics of the water mass that is subject to diabatic
671 changes: wind stress effect is rescaled by $Z(\rho)$ and mixing by $\partial_\rho Z(\rho)$. This
672 can lead to strong differences with respect to the traditional Ertel PV form,
673 for instance in region of ventilation, where a water mass is subject to heat

674 and momentum forcing at the surface before subducting and filling a deep
675 layer.

676 Note that the evolution equation 6 is valid for other choices of the refer-
677 ence density profile, for instance using a "local" -but time evolving- reference
678 density profile chosen at a fixed position. In this case, the interpretation of
679 the PV evolution is different, relative to the PV and circulation fields at
680 the chosen location. In the numerical configuration tested here, a choice of
681 a reference profile chosen in the middle of the basin yielded similar results
682 (not shown). In previous studies (Delpech et al., 2020; Assene et al., 2020;
683 Aguedjou et al., 2021; Napolitano et al., 2022; Ernst et al., 2023) we chose a
684 profile in the area of interest and fixed in time, arguing that, since we con-
685 centrated on the dynamics of deep layers, the reference stratification does
686 not evolve much. Thus simpler choices for the reference profile are possible,
687 but the ideal and rigorous choice remains Lorenz's rearranged profile.

688 The calculation of Lorenz's profile is generally straightforward and differ-
689 ent methodologies have been proposed (Winters and D'Asaro, 1996; Tseng
690 and Ferziger, 2001; Tailleux, 2013b). However, specific configurations may
691 require adaptations, such as the periodic channel one used here. Other
692 possible difficulties may arise from realistic configurations over a restricted
693 region forced at its boundaries by fluxes from a larger domain. If the water
694 mass characteristics entering the region varies, the interpretation of the PV
695 evolution based on the rearranged profile in the region can be more difficult.
696 For instance, in the present configuration, we mimicked open boundaries by
697 restricting the calculation of the rearranged profile to the Northern half of
698 the basin. We found this can lead to some biases in PV production by mix-
699 ing. Indeed, because of the transverse circulation associated with the upwelling
700 development leads to light layers depletion and deep layers inflation, the

701 reference profile evolves even when there is no mixing. Interpretation of the
702 PV evolution must then be made with care.

703 We then numerically evaluate the use of this PV formulation using a
704 simplified configuration of an upwelling developing in a periodic channel. In
705 the reference upwelling simulation, with a strong mean wind, both diapycnal
706 mixing and friction influence the PV evolution of particles. Outcropping of
707 isopycnals at the surface provides the main reservoir for cyclonic eddy gen-
708 eration (Bretherton, 1966; Morel et al., 2006). Interior diabatic effects asso-
709 ciated with friction or mixing also create positive PV anomaly eddies, but
710 the latter are generated after the onset of the instability and remain weak.
711 They play little role in the early stages of the instability. On the contrary,
712 anticyclonic vortices are associated with the generation of interior negative
713 PV anomalies, which require non-conservative effects. Prior to the onset
714 of the geostrophic instability, the friction associated with the wind stress
715 generates negative PV anomalies and the interior PV is predominantly neg-
716 ative. Mixing generates both positive and negative PV anomalies, with a net
717 effect toward positive, only partially compensating the negative generation
718 by friction. This explains the initial PV structure of the upwelling and its
719 destabilization at geostrophic scales.

720 As the instability develops, the stratification and velocity fields become
721 complex and modulate the effect of mixing and friction at small scales,
722 leading to strong changes in the PV structure. At this stage, implicit diss-
723 ipation associated with numerical schemes becomes influential and spoils the
724 PV budget when using the explicit friction and mixing terms.

725 For a lower intensity of the wind stress, the effect of friction remains
726 similar with a negative production, but at a lower rate. On the other hand,
727 the effect of mixing is strongly modified: higher stratification associated with

728 the upwelling development under a weaker wind leads to less intense mixing
729 in the upwelling region than in the open ocean and a net negative production
730 rate for the rescaled PV. The global PV production due to mixing is an order
731 of magnitude smaller than that due to friction. This shows the sensitivity of
732 PV modification by non-conservative processes and their parameterizations.

733 A downwelling develops along the southern boundary and PV is also
734 modified in this area, but the current remains stable in our configuration,
735 so we did not focus on this area. In more realistic configurations, capes or
736 topographic variations along the coast may generate localized eddies that are
737 necessarily associated with the generation of PV anomalies. It is interesting
738 to evaluate the influence of non-conservative processes in such a situation.
739 Discrepancies between the characteristics of such eddies in models and in
740 nature could well be associated with erroneous PV production associated
741 with closure schemes.

742 More generally, the present study emphasizes that parameterizations
743 play an important role in the determination of PV, the subsequent charac-
744 teristics of the eddies and the structuring of the large scale circulation (which
745 is partly determined by the redistribution of PV by the eddies). Testing dif-
746 ferent closure schemes, or parameters within a closure scheme, from the
747 perspective of PV is therefore very informative. For example, recent stud-
748 ies have shown that accounting for the modulation of the wind stress by
749 the surface ocean current feedback to the atmosphere drastically improves
750 the surface eddy properties (Renault et al., 2016b, 2020). In upwelling sys-
751 tems, the wind drop-off near the coast (Capet et al., 2004; Renault et al.,
752 2016a) or wind acceleration near capes modulates the surface stress, which,
753 combined with the vertical redistribution of momentum by the turbulent
754 fluxes, can lead to more complex effects of the wind stress (Kessouri et al.,

755 2022). It is also possible to refine the analysis and to distinguish specific
756 non-conservative effects on PV evolution (e.g. separating vertical momen-
757 tum fluxes from horizontal ones, or separating different diapycnal mixing
758 processes). All of these mechanisms, and many more, could benefit from an
759 analysis of PV generation associated with friction, mixing and their depen-
760 dence on parameterization choices. The tools we have presented here can
761 be very helpful for this perspective.

762 We have seen that when the dynamics becomes fully turbulent, there
763 are discrepancies between the PV evolution and its reconstruction from the
764 tendency terms. Temporal sub-sampling is one issue. It can be addressed by
765 on-line Lagrangian diagnostics of PV, but the strategy for the initial particle
766 positioning may be difficult, and backtracking of particles remains necessary
767 to analyze the generation of PV for a particular region or eddy. We have also
768 cited the imperfections of numerical schemes, which lead to non-conservative
769 terms that can affect the PV evolution at the grid scale, when the dynamics
770 generates small scale structures (filaments or other submesoscale eddies).
771 If these uncertainties seem to cancel out when averaging many particles in
772 the moderate wind experiment, we have seen that there is a bias possibly
773 associated with this effect in the strong wind -reference- experiment. This
774 can be problematic in achieving correct properties for eddies in numerical
775 models, but again, the tools we have proposed can help to identify numerical
776 effects and test the influence of improved numerical schemes.

777 Finally, Lorenz's profile corresponds to the minimum energy state which
778 is linked to the available potential energy (APE). In some previous studies,
779 we discussed a link between the PV structure of vortices or jets and their
780 energy (Morel and McWilliams, 2001; Morel et al., 2019). The fact that,
781 to get a rescaled PV related to the circulation, Lorenz's rearranged profile

782 is the ideal choice is thus probably not chance. The relationship between
783 rescaled PV and APE in general is thus worth investigating and some studies
784 dedicated to APE can be of great interest to substantiate the definition of the
785 ideal PV form and also possibly to identify other sources of PV modification.
786 For instance, Scotti and Passaggia (2019) have shown that the choice of
787 the Lorenz's rearranged profile to define APE can be justified because in
788 this case the effective energy does not depend on the time evolution of the
789 restratified flow, and argument that has strong similarities with the one used
790 here for the necessity of taking into account time evolution of the reference
791 profile for the rescaled PV. Finally, depending on the form of the equation
792 of state, the calculation of the Lorenz's profile is not straightforward, and
793 thermobaric effects can also make PV analysis more complicated (Straub,
794 1999). Recent studies in this field (Tailleux, 2013a,b; Saenz et al., 2015;
795 Tailleux, 2018) offer an interesting perspective for the use of PV analysis in
796 realistic configurations and are worth pursuing.

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803 lead to a much better and more rigorous manuscript.

804 **Appendix A. Numerical calculation of the reference density pro-**
805 **file**

806 Calculating Lorenz’s rearranged density profile can be efficiently done
807 by computing the pdf of the density field (Tseng and Ferziger, 2001) or
808 other methods proposed in the litterature (see for instance Tailleux, 2013b).
809 The pdf of density is easily calculated by defining fixed density classes and
810 using the density values in existing numerical cells of the configuration. The
811 obtained distribution should not suffer from biases when sigma levels and
812 density fields vary over the domain because of a varying bottom topography
813 and/or a complex -realistic- circulation is considered.

814 However, in the present configuration, we start from rest, with flat isopyc-
815 nal over a flat topography. Discarding mixing, so that the initial linear ref-
816 erence profile should be maintained, the stratification evolution consists in
817 bending isopycnals in narrow regions near the domain boundaries. In such
818 a circumstance, the density pdf might be strongly biased, with large classes
819 associated with density values over the middle of the domain and that are
820 almost unchanged with respect to the initial state, and small classes asso-
821 ciated with the slight variation near the boundaries. Such a pdf results in
822 staircase like stratification instead of the linear one, which is very problem-
823 atic for the evaluation of the rescaled PV. To avoid this problem, the existing
824 methodologies to calculate the rearranged profile was adapted as follows:

- 825 1. Define the variation of volume and surface with depth, from the surface
826 to the bottom of the domain, as a function of the vertical position z ,
827 with high enough discretization ($\Delta z \simeq 0.1 \text{ m}$). For our flat bottom
828 configuration, this is trivial.
- 829 2. Define intervals of density (density classes) covering the whole range

830 of densities present in the domain. The density range of each interval
 831 should be very small because we want to represent very small variations
 832 in the mixed layer. Here, to achieve good comparisons between direct
 833 calculation of the PV evolution rates and the one reconstructed from
 834 the tendency terms, we had to chose $\Delta\rho = 10^{-5} \text{ kg/m}^{-3}$.

- 835 3. Calculate the density pdf: affect each density cell of the 3D domain to
 836 a density class and affect its volume to the class. This is the stage when
 837 adaptations are necessary to avoid biases for the present configuration.
 838 For each horizontal position, we interpolate the density profile on a
 839 virtual vertical grid with higher resolution. This allows to refine the
 840 pdf but is more computationally demanding. To achieve good results,
 841 the vertical step we had to choose for the present configuration is
 842 $\Delta z = 0.1 \text{ m}$.
- 843 4. Calculate the net volume and mean density of each class and construct
 844 the initial rearranged 1D density profile filling the ocean from top and
 845 using the 1D volume and surface vectors determined at stage 1.
- 846 5. Interpolate the obtained profile using a regular density spacing (again
 847 a density step $\Delta\rho = 10^{-5} \text{ kg/m}^{-3}$ is necessary here) to define the
 848 rescaling function at time t $Z(\rho, t)$.

849 **Appendix B. Generalized PV evolution equation**

The traditional Ertel PV is defined as

$$PV_{Ertel} = -(\vec{\nabla} \times \vec{U} + \vec{f}) \cdot \vec{\nabla} \rho \quad (\text{B.1})$$

where \vec{U} is the velocity field, \vec{f} is the Earth rotation vector, whose projection on the local vertical axis defines the Coriolis parameter f , and ρ is the

potential density. As already mentioned by Ertel (1942) (see also Muller, 2006; Morel et al., 2019), other forms for the potential vorticity are possible, with the same adiabatic conservation properties, obtained with

$$\begin{aligned}
 PV_{rescaled} &= (\vec{\nabla} \times \vec{U} + \vec{f}) \cdot \vec{\nabla} Z(\rho) \\
 &= \vec{\nabla} \cdot ((\vec{\nabla} \times \vec{U} + \vec{f}) Z(\rho))
 \end{aligned}
 \tag{B.2}$$

850 where $Z(\rho)$ can be any function of potential density alone.

851 For geophysical flows, isopycnic variations of PV can be inverted to de-
 852 termine the geostrophic currents and associated stratification (Hoskins et al.,
 853 1985). But the Ertel PV is not the best PV expression to do so, in partic-
 854 ular, for small geostrophic perturbations relative to a state at rest, quasi-
 855 geostrophic PV (Pedlosky, 1987; Muller, 2006; Cushman-Roisin and Beck-
 856 ers, 2011) should be recovered. Indeed the quasigeostrophic PV is given
 857 by the sum of the Coriolis parameter and the 3D Laplacian of the pres-
 858 sure variations associated with the small perturbation, from which both the
 859 geostrophic current and stratification can be obtained. With this straight-
 860 forward link between PV and dynamical fields, the quasigeostrophic physics,
 861 associated with conservation and inversion of quasigeostrophic PV, provides
 862 important insights and is a fundamental approach for the understanding of
 863 the ocean dynamics from mesoscale to large scale (Pedlosky, 1987; Cushman-
 864 Roisin and Beckers, 2011). It is also at the base of the "PV thinking" ap-
 865 proach (see in particular Hoskins et al., 1985, among many other) based on
 866 the analysis of the evolution of the PV field.

867 As discussed in the introduction, to overcome some problems associated
 868 with PV_{Ertel} and simplify its interpretation, Morel et al. (2019) proposed
 869 $Z(\rho^*) = z$ (where z is the vertical coordinate oriented upward), a rescal-
 870 ing function defined using a reference density profile $\rho^*(z)$ representing the

871 stratification at rest (see also Delpech et al., 2020; Assene et al., 2020). It
872 is rigorously obtained using Lorenz (1955) diabatic rearrangement, where
873 each fluid particle is classified according to its potential density and the do-
874 main is gradually uniformly filled following this stable rearrangement (see
875 also Nakamura, 1995; Winters and D’Asaro, 1996). For such a choice, the
876 rescaled PV at rest is $PV_{rescaled}^{rest} = f$. The calculation of the reference profile
877 can be cumbersome, and in general taking into account a profile which is
878 typical of the stratification of the studied region can be taken as a reference
879 to rescale the PV.

880 In the present paper, to study the vortical dynamics of the upper layer in
881 a context of rapid diabatic evolution associated with wind stress and mixing,
882 the evolution of the reference stratification has to be taken into account.

We thus define a general rescaled PV field as

$$PV_{rescaled} = \vec{\nabla} \cdot ((\vec{\nabla} \times \vec{U} + \vec{f}) Z(\rho, t)) \quad (\text{B.3})$$

883 where $Z(\rho, t)$ is now a function of both potential density and time and
884 associated with a reference profile $\rho^*(z, t)$ that is time dependent. At any
885 time, $Z(\rho^*(z, t), t) = z$, so that the rescaled PV at rest is still given by the
886 Coriolis parameter $PV_{rescaled}^{rest} = f$.

The evolution equation for $PV_{rescaled}$ is obtained from Eq. 1 and, fol-
lowing Muller (2006), we get (see also Morel et al., 2019, for the specific
divergence form we chose here)

$$\frac{d}{dt} PV_{rescaled} = \vec{\nabla} \cdot ((\vec{\nabla} \times \vec{F}) Z(\rho, t) + (\vec{\nabla} \times \vec{U} + \vec{f}) \frac{d}{dt} [Z(\rho, t)]) \quad (\text{B.4})$$

The last term can be rewritten using

$$\frac{d}{dt} Z(\rho, t) = \partial_\rho Z(\rho, t) \dot{\rho} + \partial_t Z(\rho, t) \quad (\text{B.5})$$

We now take into account the specific form chosen for the function $Z(\rho, t)$, which verifies $Z(\rho^*(z, t), t) = z$. Differentiating the latter with respect to time yields

$$\partial_\rho Z(\rho^*(z, t), t) \partial_t \rho^*(z, t) + \partial_t Z(\rho^*(z, t), t) = 0 \quad (\text{B.6})$$

or equivalently

$$\partial_t Z(\rho^*, t) = -\partial_\rho Z(\rho^*, t) \partial_t \rho^* \quad (\text{B.7})$$

from which we get

$$\partial_t Z(\rho, t) = -\partial_\rho Z(\rho, t) \partial_t \rho^*(Z(\rho, t), t) \quad (\text{B.8})$$

Using Eq. B.8 into B.5 and finally replacing terms in B.4 we get

$$\begin{aligned} \frac{d}{dt} PV_{rescaled} = \vec{\nabla} \cdot (\vec{\nabla} \times \vec{F}) Z(\rho, t) \\ + (\vec{\nabla} \times \vec{U} + \vec{f}) \partial_\rho Z(\rho, t) (\dot{\rho} - \partial_t \rho^*(Z(\rho, t), t)) \end{aligned} \quad (\text{B.9})$$

or in Eulerian form

$$\begin{aligned} \partial_t PV_{rescaled} = \vec{\nabla} \cdot (\vec{U} PV_{rescaled} \\ + (\vec{\nabla} \times \vec{F}) Z(\rho, t) \\ + (\vec{\nabla} \times \vec{U} + \vec{f}) \partial_\rho Z(\rho, t) (\dot{\rho} - \partial_t \rho^* |_{\rho,t}) \end{aligned} \quad (\text{B.10})$$

887 where the first term of the right hand side divergence is associated with
888 adiabatic advection, the second term with friction and the third one with
889 diapycnal mixing. For the latter term, a correction is made for the gener-
890 alized rescaled PV we propose here : the diabatic mixing term has to be
891 corrected and the evolution of the reference profile $\partial_t \rho^* |_{\rho,t} = \partial_t \rho^*(Z(\rho, t), t)$
892 has to be withdrawn as it has no consequence on the generation of "dynam-
893 ical" PV anomalies. Note it has to be evaluated using the reference profile

894 time evolution at a vertical level corresponding to the density value in the
 895 physical domain (not the elevation).

896 **Appendix C. Calculation of PV and tendency terms**

897 Morel et al. (2019) showed that the divergence form of PV (Eq. 5)
 898 preserves budgets and drastically simplifies the numerical calculation of PV,
 899 which can be expressed with a compact scheme, i.e. using a single PV
 900 grid cell on a 3D Arakawa C-grid (see Fig. C.16 and Arakawa and Lamb,
 901 1977). As mentioned above, if we note the similarity between the divergence
 902 expression of PV (Eq. 5) and the diabatic PV tendency terms of its evolution
 903 equation (Eq. 6), we can see that the same scheme can be used to calculate
 904 the friction and mixing tendency terms.

Indeed, all terms can be written as

$$Div^{PV} = \vec{\nabla} \cdot (\vec{\nabla} \times \vec{F}^{vel} Z^\rho) \quad (C.1)$$

905 where Div^{PV} is the divergence calculated at PV points of the staggered
 906 C-grid (see Fig. C.16), Z^ρ is a function of density calculated at density
 907 points and $\vec{\nabla} \times \vec{F}^{vel}$ is the curl of a 3D vector $\vec{F}^{vel} = (F^U, F^V, F^W)$ whose
 908 components are located at (U, V, W) points.

Integrating Eq. C.1 over the PV cell, whose corners are located at density
 points (see Fig. C.16), we get

$$\delta V^{PV} Div^{PV} = \oint_S Z^\rho \vec{\nabla} \times \vec{F}^{vel} \cdot d\vec{S} \quad (C.2)$$

where δV^{PV} is the volume of the PV cell and the right hand side integral
 is the flux of $Z^\rho \vec{\nabla} \times \vec{F}^{vel}$ through all sides of the cell. Using the Stokes
 circulation theorem, the calculation of the latter term is simplified for the

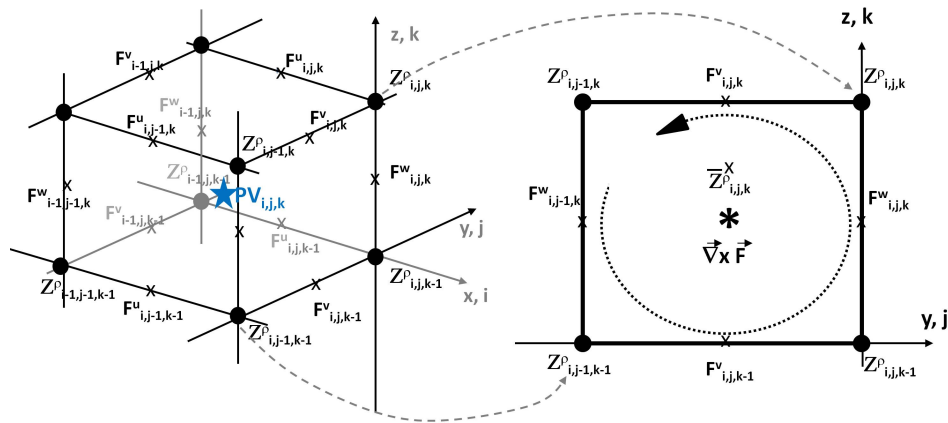


Figure C.16: Elementary cell, for a 3D C-grid, used for the calculation of PV and the tendency terms. We consider Cartesian coordinates (x, y, z) associated with indices (i, j, k) . Note that the calculation of the flux through each side of the cell is simplified for the C-grid because we can use the Stokes circulation theorem.

C-grid where velocity points are located at the center of edges parallel to the velocity component (see Fig. C.16). For instance, the flux through the side given in Fig. C.16 (right panel) is

$$\left[\oiint_S Z^\rho \vec{\nabla} \times \vec{F}^{vel} \cdot d\vec{S} \right]_{i,j,k}^x = \overline{Z^\rho}^x_{i,j,k} \cdot (F_{i,j-1,k}^W \cdot \delta z - F_{i,j,k}^W \cdot \delta z + F_{i,j,k}^V \cdot \delta y - F_{i,j,k-1}^V \cdot \delta y) \quad (\text{C.3})$$

with

$$\overline{Z^\rho}^x_{i,j,k} = \frac{Z_{i,j,k}^\rho + Z_{i,j,k-1}^\rho + Z_{i,j-1,k}^\rho + Z_{i,j-1,k-1}^\rho}{4} \quad (\text{C.4})$$

909 and so on for the fluxes through other sides.

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